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Abstract perturbed Krylov methods

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Abstract

We introduce the framework of "abstract perturbed Krylov methods". This is a new and unifying point of view on Krylov subspace methods based solely on the matrix equation $AQ_k + F_k = Q_{k+1}\underline{C}_k = Q_kC_k + q_{k+1}c_{k+1,k}e_k^{\mathrm{T}}$ and the assumption that the matrix C_k is unreduced Hessenberg. We give polynomial expressions relating the Ritz vectors, quasi-orthogonal residual iterates and quasi-minimal residual iterates to the starting vector q_1 and the perturbation term F_k. The properties of these polynomials and similarities between them are analyzed in some detail. The results suggest the interpretation of abstract *perturbed* Krylov methods as additive overlay of several abstract *exact* Krylov methods.

AMS classification: 15A24 (primary); 65Y20; 15A15; 65F10; 65F15; 65F20

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1. Introduction

We consider the matrix equation

$$AQ_k + F_k = Q_{k+1}\underline{C}_k = Q_kC_k + M_k = Q_kC_k + q_{k+1}c_{k+1,k}e_k^{\mathrm{T}}, \tag{1.1}$$

and thus implicitly every perturbed Krylov subspace method that can be written in this form. We refer to Eq. (1.1) as a *perturbed Krylov decomposition* and think of any instance of such an equation as stemming from an *abstract perturbed Krylov method*. In the remainder of the introduction we

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clarify the rôle the particular ingredients take in this perturbed Krylov decomposition, motivate the present note and introduce notations.

The matrix $A \in \mathbb{C}^{n\times n}$ is a given matrix. In Sections 4 and 5 it is the system matrix of a linear system of equations with given right-hand side b, approximate solution x_0, and thus residual r_0,

$$Ax = b - Ax_0 = r_0. \tag{1.2}$$

We restrict ourselves to the case of regular A, the case of singular A is treated in [50]. In Section 3 we are interested in some of its eigenvalues and maybe the corresponding eigenvectors, thus we consider the approximation of eigenpairs (λ, v),

$$Av = v\lambda. \tag{1.3}$$

The matrix $Q_k \in \mathbb{C}^{n\times k}$ and its expanded counterpart $Q_{k+1} \in \mathbb{C}^{n\times(k+1)}$ collect as column vectors the vectors $q_1, q_2, \ldots, q_k \in \mathbb{C}^n$ (and $q_{k+1} \in \mathbb{C}^n$). In some of the methods under consideration, these vectors form at least in some circumstances a basis of the underlying unperturbed Krylov subspace $\mathscr{K}_k$, defined by setting $q = q_1$ and

$$\mathscr{K}_k = \mathscr{K}_k(A, q) = \operatorname{span}\{q, Aq, A^2q, \ldots, A^{k-1}q\}. \tag{1.4}$$

To smoothen the understanding process we will laxly speak in *all* cases of them as the basis vectors of the possibly perturbed Krylov subspace method. The gain lies in the simplicity of this notion; the justification is that we are seldom interested in the true basis of the unperturbed Krylov subspace and that in most cases there does not exist a nearby Krylov subspace at all, the reasons becoming obvious in Theorem 2.3.

The matrix $F_k \in \mathbb{C}^{n\times k}$ is to be considered as a perturbation term. This perturbation term may be zero; in this case all results we derive in this note remain valid and make statements about the unperturbed Krylov subspace methods. The perturbation term may be due to a balancing of the equation necessary because of execution in finite precision; in this case, the term will frequently in some sense be small and we usually have bounds or estimates on the norms of the column vectors. The term may arise from a so-called *inexact* Krylov subspace method [4,43,48]; in this case the columns $\{f_l\}_{l=1}^k$ of F_k are due to inexact matrix–vector multiplies, we have control on the norms of the perturbation terms and are interested in the upper bounds on the magnitudes that do not spoil the convergence of the method. Of course the perturbation terms in the latter two settings have to be combined when one wishes to understand the properties of inexact Krylov subspace methods executed in finite precision.

The matrix $C_k \in \mathbb{C}^{k\times k}$ is an unreduced upper Hessenberg matrix, frequently an approximation to a projection of A onto the space spanned by Q_k. The capital letter C should remind of *condensed* and, especially in the perturbed variants, *computed*. The square matrix C_k is used to construct approximations to eigenvalues and eigenvectors and, in context of QOR Krylov subspace methods, to construct approximations to the solution of a linear system. It is essential for our investigations that C_k is an unreduced upper Hessenberg matrix. Under this assumption the results proven in the particular case of an unperturbed method give expressions for the quantities of interest in terms of polynomials in A times the starting vector q, which is the link of Eq. (1.1) to Krylov subspaces, and justifies the notion of “abstract perturbed Krylov methods”.

The matrix $\underline{C}_k \in \mathbb{C}^{(k+1)\times k}$ is an *extended* unreduced upper Hessenberg matrix. The rectangular matrix $\underline{C}_k$ is used in context of QMR Krylov subspace methods to construct approximations to the solution of a linear system. The notation $\underline{C}_k$ should remind of an additional *row* which is appended to the *bottom* of the Hessenberg matrix C_k and seems to have been coined independently by Sleijpen [44] and Gutknecht [24]. We feel that this notation should be preferred against other attempts of notation like $\overline{C}_k$, $\widetilde{C}_k$ or even C_k^e.

The properties of unreduced upper Hessenberg matrices have recently been investigated in [51]; these relations are the basis for the results obtained in this paper. The results are a refinement of the results proven in the Dissertation [52]. Of course, most of the results are based on prior work of other researchers, we only want to mention explicitly some of them. The work of Stiefel [45] on residual and kernel polynomials and of Freund [18] on quasi-kernel polynomials gives the representations of residuals in terms of polynomials in the exact case; unfortunately the proofs do not carry easily over to the perturbed setting. The works [48] of van den Eshof and Sleijpen and [43] of Simoncini and Szyld on inexact Krylov subspace methods include many expressions similar to ours; the main difference is the focus on polynomials taken in this paper. The works of Paige [37,33–35], Greenbaum [21,23], Greenbaum and Strakoš [22], Bai [3], Day [13,12], Scott [39], Simon [40,41], Parlett [38], Grcar [20], Cullum and Willoughby [10,11] and Tong and Ye [47] are examples of the treatment of finite precision Krylov methods; the approaches taken in these works point out the importance of Eq. (1.1). Some of the latter are described and extended in the recent publication [31]. These pointers represent only a small subjectively chosen portion of the existing work, but unfortunately no textbook dealing in greater detail with the perturbed or at least the finite precision behavior of Krylov subspace methods does exist. The new book [30] of Meurant, which is an extension of [31], will hopefully make the material on `CG` [25] and the symmetric method of Lanczos [28] accessible to a larger audience.

1.1. Motivation

In this note we consider some of the interesting properties of quantities related to Eq. (1.1). The only and crucial assumption is that the matrix C_k is unreduced Hessenberg. The good news is that most simple Krylov subspace methods are captured by Eq. (1.1). The startling news is that additionally some methods with a rather strange behavior are also covered. For a brief account of some of the methods covered we refer to [52].

Most numerical analysts will agree that there is an interest in the proper understanding of Krylov subspace methods, especially of the finite precision and inexact variants. The exact variants are more or less well understood since [45]; polynomial representations using Hankel determinants are promoted by Brezinski and co-workers, see, e.g. [5]. Unfortunately, these approaches do not seem to easily carry over to the perturbed variants. The "usual" branch of investigation of perturbed variants picks *one* variant of *one* method for *one* task in *one* "flavor", say the *finite precision* variant of the *symmetric* method of Lanczos [28] for the solution of the partial *eigenvalue* problem, implemented in the "stablest" *variant (A1)*[1] as categorized by Paige [33,34]. The beautiful analysis relies heavily on the properties of this particular method, in the case mentioned the so-called *local orthogonality* of the computed basis vectors, the *symmetry* of the computed unreduced *tridiagonal matrices* $T_k \equiv C_k \in \mathbb{R}^{k\times k}$ and the underlying *short-term recurrence*.

The subsumption of *several* methods that are quite distinct in nature under *one* common *abstract* framework undertaken in this paper will most probably be considered to be rather strange, if not useless, or even harmful. Quoting the Merriam-Webster Online Dictionary, the verb "abstract" means "to consider apart from application to or association with a particular instance" and the adjective "abstract" means "disassociated from any specific instance". The framework developed in this paper tries to strike a balance between the benefits of such an abstraction, e.g. unification

[1] There are two different algorithms in the works of Paige, which, unfortunately, are both denoted by A1. The first occurs in his Ph.D. thesis [37] and is referred to in the book [30] by Meurant, the second algorithm occurs in [33] as A(2,7) and in [34] as A1, which is the one referred to here.

and derivation of *qualitative* results, and the loss of knowledge necessary to give any *quantitative* results, e.g. the convergence of a method in finite precision.

There are several frameworks for the taxonomy of Krylov subspace methods. We mention a few and point out why we could not use them as such. The taxonomy of Krylov subspace methods by Ashby et al. [2] and the taxonomy by Broyden [7] (see also [8]) classify linear system solvers, mostly those based on short-term recurrences. The classification is based on optimization, i.e., minimization and orthogonality, properties which are destroyed in finite precision and thus not present when subject to more general perturbations. The geometric approach using angles between subspaces by Eiermann and Ernst [15] provides a distinction of methods for the solution of linear systems into (quasi-)orthogonal residual and (quasi-)minimal residual methods. These properties do not persist in the perturbed methods; the classification [15, Section 4] using coordinates can still be used to distinguish two classes of methods. The approach by Brezinski and co-workers [5] to classify various methods related to the method of Lanczos based on formal orthogonal polynomials relies on the theoretical properties like orthogonality. These properties are no longer present in the perturbed methods. To summarize: all the categorizations mentioned above are mostly inapplicable when considering finite precision or more general perturbations. The requirements have to be relaxed to allow for perturbations; this results in the restriction that the methods and their distinction are treated solely as matrix equations or equations in terms of matrix polynomials.

The treatise by Gutknecht [24] is based on matrix equations and allows inclusion of finite precision issues, even though most part is devoted to the exact case. Perturbations in Krylov subspace methods for the solution of linear systems due to inexact matrix–vector multiplies where considered by Simoncini and Szyld in [43]. The methods where grouped into those minimizing a norm and those satisfying an orthogonality property, both when unperturbed. Their analysis is based on matrix linear algebra. Compared to our general setting their analysis is simplified, since in the case they investigated, the computed "basis" is a true (bi)orthogonal basis of a related Krylov subspace [43, Eq. (2.4), p. 456] and for "minimizing" methods a true minimization property [43, Proposition 3.2, p. 457] and for "orthogonal" methods an orthogonality relation [43, Proposition 3.3, p. 458] is satisfied. This enables the derivation of bounds for the computed residuals, whereas we give exact expressions of them. The treatment [48] by van den Eshof and Sleijpen of inexact Krylov methods for linear systems is in style similar to Gutknecht's treatise. In comparison to [43] we mention that they drop the constraint that the "basis" vectors should be (bi)orthogonal. The results presented in [48] have many similarities with the results obtained here; the main difference are the *polynomial* exact expressions obtained here and the allowance for more general perturbations. The framework used in the present paper is close to that used by Gutknecht in [24] and to that used by van den Eshof and Sleijpen in [48].

In Section 2 we give expressions for the basis vectors. In Section 3 we focus on the properties of eigenpair approximations defined by

$$(\theta, y = Q_k s), \quad \text{where } C_k s = s\theta. \tag{1.5}$$

We refer to the approximate eigenpairs (θ, y) for simplicity as Ritz pairs even in the perturbed case. We distinguish the methods to compute approximate solutions to linear systems of equations into QOR methods defined in Section 4 and QMR methods defined in Section 5. These definitions are consistent with [15, Section 4], where QOR is the abbreviation of quasi-orthogonal residual and QMR the abbreviation of quasi-minimal residual. We use the same acronyms even though most perturbed methods fail to produce (quasi-)orthogonal residuals or (quasi-)minimal residuals in the usual sense.

Below we prove that the quantities associated to Krylov subspace methods, i.e., the Ritz vectors, the QOR and QMR iterates, and their corresponding residuals and errors, of *any* Krylov subspace method returning quantities covered by Eq. (1.1) can be described in terms of polynomials related *solely* to the computed C_k or $\underline{C}_k$. These results could have been achieved without the setting of abstract perturbed Krylov methods, but focusing from the *beginning* on a particular instance, e.g. the inexact variant of the method of Arnoldi [1] or unperturbed `BiCGStab` by van der Vorst [49] clouds the view for such intrinsic properties and would presumably result in yet another large amount of articles proving essentially the same result for every particular method.

The qualitative results achieved in this paper should be considered as companion to the "classical" results; focusing on a particular instance, e.g. the aforementioned variant (A1) of the method of Lanczos executed in finite precision, we can utilize results about the convergence of Ritz values to make predictions on the expected behavior of the other quantities, e.g. the Ritz vectors and their relation to eigenvectors of A. This note hopefully stimulates a combination of the classical bottom-up investigation with the new top-down approach presented here which might give new insights. An interesting example of the co-existence of the matrix based approach and the polynomial based approach is given in the paper [31] by Meurant and Strakoš and in the new book [30] by Meurant.

1.2. Notation

As usual, $I = I_k$ denotes the identity matrix of appropriate dimensions. The columns are the standard unit vectors e_j, the elements are Kronecker delta δ_{ij}. The letter $O = O_k$ denotes a zero matrix of appropriate dimensions. Zero vectors of length j are denoted by o_j. Standard unit vectors padded with one additional zero element at the bottom are denoted by

$$\underline{e}_j \equiv \begin{pmatrix} e_j \\ 0 \end{pmatrix} \in \mathbb{C}^{k+1}, \quad e_j \in \mathbb{C}^k. \tag{1.6}$$

The identity matrix of size $k \times k$ padded with an additional zero row at the bottom is denoted by $\underline{I}_k$. The augmented versions of the Hessenberg matrix and the first standard unit vector arise naturally in the form of a least c-squares problem in the context of QMR methods. To distinguish between QOR and QMR quantities and at the same time to depict the relations between both clear-cut and easily accessible, we abuse the notation just introduced and denote all QMR quantities with a lower bar like $\underline{z}_k$, $\underline{x}_k$, $\underline{r}_k$ in contrast to z_k, x_k, r_k. Section five is mostly based on relations between QOR and QMR, so we need a clear-cut notation, and the danger of confusing extended versions of vectors with QMR quantities is diminished since the dimensions are always clear from the context. The QMR relations are *based* on the corresponding QOR results, thus the notation has to allow for a distinction between QOR and QMR quantities, yet to focus on similarities.

The characteristic matrices $zI - A$ and $zI - C_k$ are denoted by ${}^zA$ and ${}^zC_k$. The characteristic polynomials $\chi(z)$ of A and $\chi_k(z)$ of C_k are defined by $\chi(z) \equiv \det({}^zA)$ and $\chi_k(z) \equiv \det({}^zC_k)$, respectively. Let θ be an eigenvalue of C_k of algebraic multiplicity $\alpha \equiv \alpha(\theta)$. The reduced characteristic polynomial $\omega_k(z)$ of C_k corresponding to θ is defined by

$$\chi_k(z) = (z - \theta)^\alpha \omega_k(z). \tag{1.7}$$

We remark that $\omega_k(\theta) \neq 0$. We make extensive use of other characteristic polynomials denoted by $\chi_{i:j}$ and defined by

$$\chi_{i:j}(z) \equiv \det({}^zC_{i:j}) \equiv \det(zI - C_{i:j}), \tag{1.8}$$

where $C_{i:j}$ denotes the principal submatrix of C_k consisting of the columns and rows i to j, for all admissible indices $1 \leqslant i \leqslant j \leqslant k$. We extend the notation to the case $i = j + 1$ by setting $\chi_{j+1:j}(z) \equiv 1$ for all j. Additionally we define the shorthand notation $\chi_j = \chi_{1:j}$.

We denote products of subdiagonal elements of the unreduced Hessenberg matrices C_k by $c_{i:j} \equiv \prod_{l=i}^{j} c_{l+1,l}$. Polynomial vectors ν and $\check{\nu}$ are defined by

$$\nu(z) \equiv \left(\frac{\chi_{j+1:k}(z)}{c_{j:k-1}}\right)_{j=1}^{k} \quad \text{and} \quad \check{\nu}(z) \equiv \left(\frac{\chi_{1:j-1}(z)}{c_{1:j-1}}\right)_{j=1}^{k}. \tag{1.9}$$

The elements are denoted by $\nu_j(z)$ and $\check{\nu}_j(z)$, where j runs from 1 to k. The notation is extended to include the polynomial $\check{\nu}_{k+1}(z)$, defined by

$$\check{\nu}_{k+1}(z) \equiv \frac{\chi_{1:k}(z)}{c_{1:k}}. \tag{1.10}$$

We extend the polynomial vector $\check{\nu}$ by padding it in the last position with the polynomial $\check{\nu}_{k+1}$, denoted by $\underline{\check{\nu}}$,

$$\underline{\check{\nu}}(z) \equiv \begin{pmatrix} \check{\nu}(z)^{\mathrm{T}} & \check{\nu}_{k+1}(z) \end{pmatrix}^{\mathrm{T}} = \begin{pmatrix} \check{\nu}_1(z) & \cdots & \check{\nu}_k(z) & \check{\nu}_{k+1}(z) \end{pmatrix}^{\mathrm{T}}. \tag{1.11}$$

We denote the complex conjugates of $\check{\nu}$, $\check{\nu}_j$, $\underline{\check{\nu}}$ by $\hat{\nu}$, $\hat{\nu}_j$, $\underline{\hat{\nu}}$, respectively. The operation "complex conjugate" can be memorized as a reflection on the real axis turning hat to vee and vice versa.

The Jordan normal forms of A and C_k are denoted by J and J_k, respectively. Similarity transformations V and S_k are chosen to satisfy

$$V^{-1}AV = J, \quad S_k^{-1}C_kS_k = J_k. \tag{1.12}$$

We call *any* matrices V and S_k that satisfy Eq. (1.12) (*right*) *eigenmatrices* and define corresponding (special) *left eigenmatrices* by

$$\hat{V}^H \equiv \check{V}^{\mathrm{T}} \equiv V^{-1}, \quad \hat{S}_k^H \equiv \check{S}_k^{\mathrm{T}} \equiv S_k^{-1}. \tag{1.13}$$

This definition ensures the biorthogonality of left and right eigenmatrices, which is a partial normalization of the eigen- and principal vectors. When A is normal, we set $\hat{V} \equiv V$, when C_k is normal, we set $\hat{S}_k \equiv S_k$. In any of these cases the eigenvectors are normalized to have unit length, since the *bi*orthogonality simplifies to orthogonality.

The eigenvalues of A and C_k are distinguished by the Greek letters λ and θ, respectively. For reasons of simplicity, we refer to the eigenvalues θ of C_k as Ritz values. These values are *only* Ritz values of A when an underlying projection exists, but they are *always* Ritz values of $C_{k+\ell}$, for any $\ell \in \mathbb{N}$.

The Jordan matrix J of A is the direct sum of Jordan blocks. The direct sum of the γ Jordan blocks to an eigenvalue λ, where $\gamma = \gamma(\lambda)$ denotes the geometric multiplicity of λ, is called a Jordan box and denoted by J_λ. The Jordan blocks are denoted by $J_{\lambda\iota}$, where $\iota = 1, 2, \ldots, \gamma$. A single Jordan block $J_{\lambda\iota}$ has dimension $\sigma = \sigma(\lambda, \iota)$ and is *upper* triangular,

$$J_{\lambda\iota} = \begin{pmatrix} \lambda & 1 & & \\ & \lambda & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{pmatrix} = \lambda I_\sigma + N_\sigma \in \mathbb{C}^{\sigma\times\sigma}. \tag{1.14}$$

Since C_k is unreduced Hessenberg, J_k is the direct sum of Jordan boxes J_θ that collapse to Jordan blocks. These notations are summarized by

$$J = \bigoplus_{\lambda} J_\lambda, \quad J_\lambda = \bigoplus_{\iota=1}^{\gamma} J_{\lambda\iota}, \quad J_k = \bigoplus_{\theta} J_\theta. \tag{1.15}$$

We split the eigenmatrices according to the splitting of the Jordan matrices into rectangular matrices,

$$V = \bigoplus_{\lambda} V_\lambda, \quad V_\lambda = \bigoplus_{\iota=1}^{\gamma} V_{\lambda\iota}, \quad S_k = \bigoplus_{\theta} S_\theta. \tag{1.16}$$

These matrices are named *partial* eigenmatrices. Similarly, left partial eigenmatrices are defined.

The adjugate of ${}^zC_k$, i.e., the transposed matrix of cofactors of ${}^zC_k$, is sometimes denoted by $P_k(z) \equiv \operatorname{adj}({}^zC_k)$ to emphasize that this matrix is polynomial in z. The Moore–Penrose inverse of a (possibly rectangular) matrix A is denoted by $A^\dagger$. In one theorem for simplicity we use the vec-operator, denoted by $\operatorname{vec}(A)$, cf. [27, Chapter 4, Definition 4.2.9]. The norm used is always the Euclidian norm and is denoted by $\|\cdot\|$.

2. Basis transformations

In the 1950s Krylov subspace methods like the methods of Arnoldi [1] and Lanczos [28] were considered as a means to compute the leading part Q_k of a basis transformation Q that brings A to Hessenberg and tridiagonal form $C = Q^{-1}AQ$, respectively, with C_k as its leading part. Even though this property is frequently lost in finite precision and is not present in the general case, this point of view is helpful in the construction of more elaborate Krylov subspace methods.

2.1. Basis vectors

In this section we give an expression of the "basis" vectors of abstract perturbed Krylov methods that reveals the dependency on the starting vector and the perturbation terms. This result is utilized in what follows to obtain similar expressions for the other quantities of interest.

For consistency with later sections we define the *basis polynomials* of an abstract perturbed Krylov method by

$$\mathscr{B}_k(z) \equiv \frac{\chi_{1:k}(z)}{c_{1:k}} = \check{\nu}_{k+1}(z), \quad \mathscr{B}_{l+1:k}(z) \equiv \frac{\chi_{l+1:k}(z)}{c_{l+1:k}} = \frac{c_{l+1,l}}{c_{k+1,k}} \nu_l(z). \tag{2.1}$$

Theorem 2.1 (The basis vectors). *The basis vectors that correspond to a perturbed Krylov decomposition* (1.1) *can be expressed in terms of the starting vector q_1 and all perturbation terms $\{f_l\}_{l=1}^k$ as follows*:

$$q_{k+1} = \mathscr{B}_k(A)q_1 + \sum_{l=1}^{k} \mathscr{B}_{l+1:k}(A)\frac{f_l}{c_{l+1,l}}. \tag{2.2}$$

Proof. We start with the perturbed Krylov decomposition (1.1). First we insert ${}^zA \equiv zI_n - A$ and ${}^zC_k \equiv zI_k - C_k$, since $Q_k zI_k = zI_n Q_k$ and thus scalar multiples of Q_k are in the null space, to introduce a dependency on variable z,

$$M_k = Q_k(zI - C_k) - (zI - A)Q_k + F_k. \tag{2.3}$$

We use the definition of the adjugate and the Laplace expansion of the determinant to obtain

$$M_k \operatorname{adj}({}^zC_k) = Q_k \chi_k(z) - (zI - A)Q_k \operatorname{adj}({}^zC_k) + F_k \operatorname{adj}({}^zC_k). \tag{2.4}$$

We know from [51, Eq. (3.11)] that the adjugate of unreduced Hessenberg matrices satisfies

$$\operatorname{adj}({}^{z}C_k)e_1 = c_{1:k-1} \cdot \nu(z). \tag{2.5}$$

Together with Eq. (2.4) this gives the simplified equation

$$c_{k+1,k}q_{k+1} = M_k\nu(z) = \frac{q_1\chi_k(z)}{c_{1:k-1}} - (zI - A)Q_k\nu(z) + F_k\nu(z). \tag{2.6}$$

We reorder Eq. (2.6) slightly to obtain an equation where only scalar polynomials are involved:

$$c_{k+1,k}q_{k+1} = \frac{\chi_k(z)q_1}{c_{1:k-1}} + \sum_{l=1}^{k}\nu_l(z)Aq_l - \sum_{l=1}^{k}\nu_l(z)zq_l + \sum_{l=1}^{k}\nu_l(z)f_l. \tag{2.7}$$

Substituting A for z gives

$$\frac{\chi_k(A)q_1}{c_{1:k-1}} + \sum_{l=1}^{k}\nu_l(A)f_l = c_{k+1,k}q_{k+1}, \tag{2.8}$$

which is upon division by nonzero $c_{k+1,k}$, a corresponding cosmetic division by nonzero $c_{l+1,l}$, $l = 1, \ldots, k$ and by definition of $\nu(z)$ the result to be proved. □

This result has been obtained for the symmetric method of Lanczos by other authors, we explicitly mention the thesis [20] by Grcar and the book [10] by Cullum and Willoughby. In his thesis [20], Grcar has used this result and bounds on the polynomials involved to develop his method of periodic reorthogonalization. Using the three-term recurrence formulation of the basis polynomials in the symmetric method of Lanczos this can also be found in the more recent paper [31, Lemma 4.12, Theorem 4.13] and book [30, Lemma 4.5, Theorem 4.6], where the latter also cites [50].

2.2. *A closer look*

In the sequel we need some additional knowledge from [51] on Hessenberg eigenvalue–eigenmatrix relations. The next lemma states a relation important in the proofs to follow. We remark that this lemma can not be found 'as is' in [51].

Lemma 2.2 (Hessenberg eigenvalue–eigenmatrix relations). *Let C_k be unreduced upper Hessenberg. Then we can choose the eigenmatrices S_k and $\check{S}_k$ such that the partial eigenmatrices satisfy*

$$e_1^{\mathrm{T}}\check{S}_\theta = e_\alpha^{\mathrm{T}}(\omega_k(J_\theta))^{-\mathrm{T}} \quad \text{and} \quad S_\theta^{\mathrm{T}}e_l = c_{1:l-1}\chi_{l+1:k}(J_\theta)^{\mathrm{T}}e_1. \tag{2.9}$$

The Hessenberg eigenvalue–eigenmatrix relations tailored to diagonalizable C_k state that

$$\check{s}_{lj}s_{\ell j} = \frac{\chi_{1:l-1}(\theta_j)c_{l:\ell-1}\chi_{\ell+1:k}(\theta_j)}{\chi_{1:k}'(\theta_j)} \quad \forall l \leqslant \ell. \tag{2.10}$$

Proof. The choice mentioned above corresponds to [51, Eq. (3.37)] with $c_{1:k-1}$ brought from the right to the left and is given by

$$S_\theta \equiv c_{1:k-1}\mathscr{V}_{\alpha-1}(\theta), \quad \check{S}_\theta \equiv \check{\mathscr{V}}_{\alpha-1}(\theta)\omega_k(J_\theta)^{-\mathrm{T}}, \tag{2.11}$$

where the unknown quantities are defined in [51, Eqs. (3.30), (3.3)] and are given by

$$\mathscr{V}_{\alpha-1}(\theta) \equiv \left(\nu(\theta), \nu'(\theta), \frac{\nu''(\theta)}{2}, \ldots, \frac{\nu^{(\alpha-1)}(\theta)}{(\alpha-1)!}\right), \tag{2.12}$$

$$\check{\mathscr{V}}_{\alpha-1}(\theta) \equiv \left(\frac{\check{\nu}^{(\alpha-1)}(\theta)}{(\alpha-1)!}, \ldots, \frac{\check{\nu}''(\theta)}{2}, \check{\nu}'(\theta), \check{\nu}(\theta) \right). \tag{2.13}$$

By definition of ν and $\check{\nu}$ it is easy to see that

$$\begin{aligned} e_1^{\mathrm{T}} \check{S}_\theta &= e_1^{\mathrm{T}} \check{\mathscr{V}}_{\alpha-1}(\theta)(\omega_k(J_\theta))^{-\mathrm{T}} = e_\alpha^{\mathrm{T}}(\omega_k(J_\theta))^{-\mathrm{T}}, \\ e_l^{\mathrm{T}} S_\theta &= c_{1:k-1} e_l^{\mathrm{T}} \left(\nu(\theta), \nu'(\theta), \frac{\nu''(\theta)}{2}, \ldots, \frac{\nu^{(\alpha-1)}(\theta)}{(\alpha-1)!} \right) \qquad (2.14) \\ &= \frac{c_{1:k-1}}{c_{l:k-1}} \left(\chi_{l+1:k}(\theta), \chi'_{l+1:k}(\theta), \frac{\chi''_{l+1:k}(\theta)}{2}, \ldots, \frac{\chi^{(\alpha-1)}_{l+1:k}(\theta)}{(\alpha-1)!} \right). \qquad (2.15) \end{aligned}$$

The row vector $e_l^{\mathrm{T}} S_\theta / c_{1:l-1}$ consists of Taylor expansion terms that can also be written as

$$\left(\chi_{l+1:k}(\theta), \chi'_{l+1:k}(\theta), \frac{\chi''_{l+1:k}(\theta)}{2}, \ldots, \frac{\chi^{(\alpha-1)}_{l+1:k}(\theta)}{(\alpha-1)!} \right) = e_1^{\mathrm{T}} \chi_{l+1:k}(J_\theta),$$

i.e., interpreted as the first row of the polynomial $\chi_{l+1:k}$ evaluated at the Jordan block J_θ. The statement in Eq. (2.10) is just a rewritten version of [51, Theorem 3.6, Eq. (3.31)]. □

In most cases we will compute diagonalizable matrices and are interested in eigenvectors solely. In the following, we refer to the coefficients of a vector in the eigenbasis, i.e., in the basis spanned by the columns of V, as its eigenparts. The next theorem generalizes some expressions obtained by Paige [35] for the symmetric method of Lanczos to our abstract setting. Paige related loss of orthogonality using known error bounds to expressions based on three different conditions involving solely the Ritz values and eigenvectors of C_j, $1 \leqslant j \leqslant k$. In contrast to Paige's theory we can only give conditions for amplifications of the eigenparts of the basis vectors, which are additionally based on unknown data like eigenvalues and eigenvectors of A. Similar to Paige's theory the amplification is related to different conditions. In our abstract setting these are: a small residual estimator, the convergence of a Ritz value to an eigenvalue, and the closeness of at least two Ritz values.

Theorem 2.3 (The eigenparts of the basis vectors). *Let $\hat{v}^H$ be a left eigenvector of A to eigenvalue λ and let s be a right eigenvector of C_k to eigenvalue θ.*

Then the eigenpart $\hat{v}^H q_{k+1}$ of the basis vector q_{k+1} of a perturbed Krylov decomposition (1.1) *can be expressed in terms of the Ritz value θ and the Ritz vector $y \equiv Q_k s$ as follows*:

$$\hat{v}^H q_{k+1} = \frac{(\lambda - \theta)\hat{v}^H y}{c_{k+1,k} e_k^{\mathrm{T}} s} + \frac{\hat{v}^H F_k s}{c_{k+1,k} e_k^{\mathrm{T}} s}. \tag{2.16}$$

Let furthermore C_k be diagonalizable and suppose that $\lambda \neq \theta_j$ for all $j = 1, \ldots, k$.

Then we can express the dependency of the eigenpart $\hat{v}^H q_{k+1}$ of q_{k+1} on the starting vector q_1 and the perturbation terms $\{f_l\}_{l=1}^k$ in three equivalent forms. In terms of the distances of the Ritz values θ_j to λ and the left and right eigenvectors of the matrix C_k:

$$\left(\sum_{j=1}^k \frac{c_{k+1,k} \check{s}_{1j} s_{kj}}{\lambda - \theta_j} \right) \hat{v}^H q_{k+1} = \hat{v}^H q_1 + \sum_{l=1}^k \left(\sum_{j=1}^k \frac{c_{l+1,l} \check{s}_{1j} s_{lj}}{\lambda - \theta_j} \right) \frac{\hat{v}^H f_l}{c_{l+1,l}}. \tag{2.17}$$

In terms of the distances of the Ritz values to λ, *the trailing characteristic polynomials of* C_k *and the derivative of the characteristic polynomial of* C_k, *all evaluated at the Ritz values*:

$$\left(\sum_{j=1}^{k}\frac{c_{1:k}}{\chi'_{1:k}(\theta_j)(\lambda-\theta_j)}\right)\hat{v}^H q_{k+1}=\hat{v}^H q_1+\sum_{l=1}^{k}\left(\sum_{j=1}^{k}\frac{c_{1:l}\chi_{l+1:k}(\theta_j)}{\chi'_{1:k}(\theta_j)(\lambda-\theta_j)}\right)\frac{\hat{v}^H f_l}{c_{l+1,l}}. \tag{2.18}$$

Without the restriction on λ, *in terms of trailing characteristic polynomials of* C_k *evaluated at the eigenvalue* λ *of* A:

$$\hat{v}^H q_{k+1}=\left(\frac{\chi_{1:k}(\lambda)}{c_{1:k}}\right)\hat{v}^H q_1+\sum_{l=1}^{k}\left(\frac{\chi_{l+1:k}(\lambda)}{c_{l+1:k}}\right)\frac{\hat{v}^H f_l}{c_{l+1,l}}. \tag{2.19}$$

Proof. We multiply Eq. (1.1) from the left by $\hat{v}^H$ and from the right by s and obtain

$$\hat{v}^H q_{k+1}c_{k+1,k}e_k^{\mathrm{T}}s=(\lambda-\theta)\hat{v}^H y+\hat{v}^H F_k s. \tag{2.20}$$

The constant $c_{k+1,k}$ is nonzero because C_k is unreduced Hessenberg. The last component of s is nonzero because s is a right eigenvector of an unreduced Hessenberg matrix [51, Corollary 3.2]. Eq. (2.16) follows upon division by $c_{k+1,k}e_k^{\mathrm{T}}s$.

When C_k is diagonalizable, the columns of the eigenmatrix S_k form a complete set of eigenvectors s_j, $j=1,\ldots,k$. We use this basis to express the standard unit vectors e_ℓ by use of the following (trivial) identity:

$$e_\ell=Ie_\ell=SS^{-1}e_\ell=S\check{S}^{\mathrm{T}}e_\ell=\sum_{j=1}^{k}\check{s}_{\ell j}s_j \tag{2.21}$$

Eq. (2.20) holds true for all pairs (θ_j,s_j). We assume that $\lambda\neq\theta_j$ for all Ritz values θ_j and divide by $\lambda-\theta_j$ to obtain the following set of equations:

$$\left(\frac{c_{k+1,k}s_{kj}}{\lambda-\theta_j}\right)\hat{v}^H q_{k+1}=\hat{v}^H Q_k s_j+\sum_{l=1}^{k}\left(\frac{c_{l+1,l}s_{lj}}{\lambda-\theta_j}\right)\frac{\hat{v}^H f_l}{c_{l+1,l}},\quad j=1,\ldots,k. \tag{2.22}$$

Here we have chosen for cosmetic reasons to divide by $c_{l+1,l}$ in the perturbation terms. All $c_{l+1,l}$ are nonzero since the Hessenberg matrix C_k is unreduced. We sum up the equations (2.22) using the identity (2.21) for the case $\ell=1$ to obtain (2.17). We insert the Hessenberg eigenvalue–eigenmatrix relations tailored to diagonalizable C_k given by Lemma 2.2, Eq. (2.10) into the first term of (2.17) and obtain

$$\left(\sum_{j=1}^{k}\frac{c_{1:k}}{\chi'_{1:k}(\theta_j)(\lambda-\theta_j)}\right)\hat{v}^H q_{k+1}=\hat{v}^H q_1+\sum_{l=1}^{k}\left(\sum_{j=1}^{k}\frac{c_{l+1,l}\check{s}_{1j}s_{lj}}{\lambda-\theta_j}\right)\frac{\hat{v}^H f_l}{c_{l+1,l}}. \tag{2.23}$$

When we insert Eq. (2.10) in repeated manner into the second term of Eq. (2.17) we obtain (2.18). Now it is time to recognize that an expression like

$$\sum_{j=1}^{k}\frac{f(\theta_j)}{\chi'_{1:k}(\theta_j)(\lambda-\theta_j)}=\frac{1}{\chi_{1:k}(\lambda)}\sum_{j=1}^{k}\frac{\prod_{s\neq j}(\lambda-\theta_s)}{\prod_{s\neq j}(\theta_j-\theta_s)}f(\theta_j) \tag{2.24}$$

is just the Lagrange form of the interpolation of a function f at nodes $\{\theta_j\}_{j=1}^k$ divided by constant $\chi_{1:k}(\lambda)$. Recognizing that the first term is the interpolation of the constant function $f \equiv 1$ at the Ritz values, we obtain

$$\left(\frac{c_{1:k}}{\chi_{1:k}(\lambda)}\right)\hat{v}^H q_{k+1} = \hat{v}^H q_1 + \sum_{l=1}^k \left(\sum_{j=1}^k \frac{c_{1:l}\,\chi_{l+1:k}(\theta_j)}{\chi'_{1:k}(\theta_j)(\lambda-\theta_j)}\right)\frac{\hat{v}^H f_l}{c_{l+1,l}}. \tag{2.25}$$

The repeated use of this argument for the second term shows that this is the Lagrange interpolation of the polynomials $\chi_{l+1:k}$ of degrees less than k,

$$\left(\frac{c_{1:k}}{\chi_{1:k}(\lambda)}\right)\hat{v}^H q_{k+1} = \hat{v}^H q_1 + \sum_{l=1}^k \left(\frac{c_{1:l}\,\chi_{l+1:k}(\lambda)}{\chi_{1:k}(\lambda)}\right)\frac{\hat{v}^H f_l}{c_{l+1,l}}. \tag{2.26}$$

Division by the first factor results in (2.19). It follows from Theorem 2.1 by multiplication of Eq. (2.2) from the left by $\hat{v}^H$ that Eq. (2.19) remains valid without any artificial restrictions on the eigenvalue λ and without the need for a diagonalizable Hessenberg matrix C_k. □

The validity of Theorem 2.1 for general matrices A and *general* unreduced Hessenberg matrices C_k suggests that we can also derive expressions for the eigenparts in the general (i.e., not necessarily diagonalizable) case. This rather technical part is omitted for sake of simplicity, but is part of the underlying technical report [50].

3. Eigenvalue problems

In the last section we have shown how the convergence of the Ritz values to an eigenvalue results in the amplification of the error terms. Thus, the convergence of the Ritz values affects the amplification of perturbation terms, which affects the construction of the next basis vector, which in turn is used to compute the next elements of C_k, which defines the next set of Ritz values. The resulting nonlinearity of the convergence behavior of Ritz values to eigenvalues of A reveals that it is hopeless to ask for results on the convergence of the Ritz values, at least in this abstract setting. One branch of investigation uses the properties of the constructed basis vectors, e.g. (local) orthogonality, to make statements about the convergence of Ritz values. We simply drop the convergence analysis for the Ritz *values* and ask for expressions revealing conditions for a convergence of the Ritz *vectors* and Ritz *residuals*.

Residuals directly give information on the backward errors of the corresponding quantities. The removal of the dependency on the condition that is related to the forward error makes the Ritz residuals slightly more appealing as a point to start the examination.

3.1. Ritz residuals

The analysis of the Ritz residuals is simplified since we can easily compute an a posteriori bound involving the next basis vector q_{k+1}. Adding the expression for the basis vectors of the last section we can prove the following theorem.

Theorem 3.1 (The Ritz residuals). *Let θ be an eigenvalue of C_k with Jordan block J_θ and S_θ any corresponding partial eigenmatrix. Define the partial Ritz matrix by $Y_\theta \equiv Q_k S_\theta$.*

Then

$$AY_\theta - Y_\theta J_\theta = \left(\frac{\chi_{1:k}(A)}{c_{1:k-1}}\right) q_1 e_k^{\mathrm{T}} S_\theta + \sum_{l=1}^{k} \left(\frac{\chi_{l+1:k}(A)}{c_{l:k-1}}\right) f_l e_k^{\mathrm{T}} S_\theta - f_l e_l^{\mathrm{T}} S_\theta. \tag{3.1}$$

Let S_θ be the (unique) partial eigenmatrix given in Lemma 2.2.
Then

$$AY_\theta - Y_\theta J_\theta = \chi_{1:k}(A) q_1 e_1^{\mathrm{T}} + \sum_{l=1}^{k} c_{1:l-1} \Big(\chi_{l+1:k}(A) f_l e_1^{\mathrm{T}} - f_l e_1^{\mathrm{T}} \chi_{l+1:k}(J_\theta)\Big). \tag{3.2}$$

Proof. We start with the backward expression for the Ritz residual

$$AY_\theta - Y_\theta J_\theta = q_{k+1} c_{k+1,k} e_k^{\mathrm{T}} S_\theta - \sum_{l=1}^{k} f_l e_l^{\mathrm{T}} S_\theta. \tag{3.3}$$

obtained from (1.1) by multiplication by S_θ. A scaled variant of the result in Eq. (2.2) of Theorem 2.1 is used to replace the next basis vector, namely,

$$q_{k+1} c_{k+1,k} = \left(\frac{\chi_{1:k}(A)}{c_{1:k-1}}\right) q_1 + \sum_{l=1}^{k} \left(\frac{\chi_{l+1:k}(A)}{c_{l:k-1}}\right) f_l. \tag{3.4}$$

Inserting Eq. (3.4) into Eq. (3.3) gives Eq. (3.1). Lemma 2.2 states that with our (special) choice of the biorthogonal partial eigenmatrices

$$e_k^{\mathrm{T}} S_\theta = (c_{1:k-1}) e_1^{\mathrm{T}}, \quad e_l^{\mathrm{T}} S_\theta = (c_{1:l-1}) e_1^{\mathrm{T}} \chi_{l+1:k}(J_\theta). \tag{3.5}$$

Inserting the expressions stated in Eq. (3.5) into Eq. (3.1) we obtain Eq. (3.2). □

The last equation, Eq. (3.2) of Theorem 3.1 shows that even though some trailing characteristic polynomials $\chi_{l+1:k}$ might be large at J_θ, the perturbation terms might nearly cancel and be small in direction of some left eigenvectors and principal vectors of A corresponding to part of a Jordan block close to J_θ. In the diagonalizable case of the symmetric method of Lanczos this might help to complement the analyses of the oscillating behavior of the residual estimators and the occurrence of multiple copies of Ritz values corresponding to the same eigenvalue given in, e.g., [35,10].

3.2. Ritz vectors

We observe that the adjugate of the family ${}^zC_k \equiv zI - C_k$ is given by the matrix $P_k(z)$ of cofactors, which is polynomial in z and simultaneously a polynomial in C_k for every fixed z. This is used in the following lemma to define a bivariate polynomial denoted by $\mathscr{A}_k(z, C_k)$, such that

$$P_k(z) = \mathscr{A}_k(z, C_k) = \operatorname{adj}({}^zC_k). \tag{3.6}$$

It is well known, see, e.g. [19,17,14,26], that whenever we insert a simple eigenvalue θ of C_k into $P_k(z)$ we obtain a multiple of the spectral projector. More generally, when the eigenvalue has multiplicity α we might consider the evaluation of the matrix $P_k(z)$ along with the derivatives up to order $\alpha - 1$ at θ to gain information about the eigen- *and* principal vectors of C_k, compare with [17, Section 3.6], [14] and for the case of unreduced Hessenberg matrices with [51, Corollary 2.1].

Lemma 3.2 (The adjugate polynomial). *Let the bivariate polynomial $\mathscr{A}_k(\theta, z)$ be defined by*

$$\mathscr{A}_k(\theta, z) \equiv \begin{cases} (\chi_k(\theta) - \chi_k(z))(\theta - z)^{-1}, & z \neq \theta, \\ \chi_k'(z), & z = \theta. \end{cases} \tag{3.7}$$

Then $\mathscr{A}_k(\theta, C_k)$ is the adjugate of the matrix $\theta I_k - C_k$.

Proof. Inserting the Taylor expansion of the polynomial χ_k at θ (at z) shows that the function given by the right-hand side is a polynomial of degree $k - 1$ in z (in θ). For θ not in the spectrum of C_k we have

$$\mathscr{A}_k(\theta, C_k) = (\chi_k(\theta) I_k - \chi_k(C_k))(\theta I_k - C_k)^{-1} \tag{3.8}$$

$$= \det(\theta I_k - C_k)(\theta I_k - C_k)^{-1} = \operatorname{adj}(\theta I_k - C_k). \tag{3.9}$$

The result for θ in the spectrum follows by continuity. □

Remark 3.1. The adjugate polynomials are closely related to the polynomials used by Lanczos in his original paper [28] to represent the eigenvectors of a matrix constructed by the algorithm now bearing his name. What we call adjugate polynomial appears without a name in Gantmacher's treatise [19, Kapitel 4.3, Seite 111, Formel (28)] published first 1954 in Russian. Later Taussky [46] published a related result.

We extend the notation to all trailing characteristic polynomials.

Definition 3.3 (*Trailing adjugate polynomials*). We define the bivariate polynomials $\mathscr{A}_{l+1:k}(\theta, z)$, $l = 1, \ldots, k$, that give the adjugate of a shifted matrix at the Ritz values of the trailing submatrices $C_{l+1:k}$ by

$$\mathscr{A}_{l+1:k}(\theta, z) \equiv \begin{cases} (\chi_{l+1:k}(\theta) - \chi_{l+1:k}(z))(\theta - z)^{-1}, & z \neq \theta, \\ \chi_{l+1:k}'(z), & z = \theta. \end{cases} \tag{3.10}$$

In the sequel we need an alternative expression for the adjugate polynomials which clearly reveals their polynomial structure. To proceed we first prove what we call the first adjugate identity (because of its close relation to the first resolvent identity) and specialize it to Hessenberg structure.

Proposition 3.4. *The adjugates of any matrix family ${}^zA$ satisfy the first adjugate identity given by*

$$(z - \theta)\operatorname{adj}({}^zA)\operatorname{adj}({}^\theta A) = \det({}^zA)\operatorname{adj}({}^\theta A) - \det({}^\theta A)\operatorname{adj}({}^zA). \tag{3.11}$$

For unreduced Hessenberg matrices C_k this implies the following important relation:

$$(z - \theta)\sum_{j=1}^{k} \chi_{1:j-1}(z)\chi_{j+1:k}(\theta) = \chi_k(z) - \chi_k(\theta). \tag{3.12}$$

Proof. We start with the obvious relation

$$(z - \theta)I = (zI - A) - (\theta I - A) = {}^zA - {}^\theta A. \tag{3.13}$$

The multiplication by the adjugates of ${}^zA$ and ${}^\theta A$ results in Eq. (3.11). Now consider the case of an unreduced Hessenberg matrix C_k. By [51, Eqs. (3.11) and (3.12)] we can rewrite the component $(k, 1)$ of the Eq. (3.11) in the lower left corner to obtain

$$(z-\theta)c_{1:k-1}\check{\nu}(z)^{\mathrm{T}}\nu(\theta) = \det({}^{z}C_k)\check{\nu}(\theta)^{\mathrm{T}}e_1 - \det({}^{\theta}C_k)e_k^{\mathrm{T}}\nu(z). \tag{3.14}$$

By definition of χ_k, $\check{\nu}$ and ν we have proven Eq. (3.12). □

Dividing Eq. (3.12) by the scalar factor $(z-\theta)$ (and taking limits) proves the following lemma for the adjugate polynomials $\mathscr{A}_k(\theta, z)$. Since trailing submatrices $C_{l+1:k}$ of unreduced Hessenberg matrices C_k are also unreduced Hessenberg matrices, the previous arguments also apply to the trailing adjugate polynomials.

Lemma 3.5. *The adjugate polynomial $\mathscr{A}_k(\theta, z)$ and the trailing adjugate polynomials $\mathscr{A}_{l+1:k}(\theta, z)$ can be expressed in polynomial terms as follows*:

$$\mathscr{A}_{l+1:k}(\theta, z) = \sum_{j=l+1}^{k} \chi_{l+1:j-1}(z)\chi_{j+1:k}(\theta), \quad l = 0, \ldots, k. \tag{3.15}$$

Their ℓth derivatives for all $\ell \geqslant 0$ with respect to θ are given by

$$\mathscr{A}^{(\ell)}_{l+1:k}(\theta, z) = \sum_{j=l+1}^{k} \chi_{l+1:j-1}(z)\chi^{(\ell)}_{j+1:k}(\theta), \quad l = 0, \ldots, k. \tag{3.16}$$

The relations (3.15) and (3.16) hold also true when z is replaced by a square matrix A, in which case we obtain a parameter dependent family of matrices along with their derivatives with respect to the parameter θ.

We remark that the relations stated in Lemma 3.5 rely strongly on the unreduced Hessenberg structure of the matrix C_k.

Theorem 3.6 (The Ritz vectors). *Let θ be an eigenvalue of C_k with Jordan block J_θ and let S_θ be the corresponding unique right eigenmatrix from Lemma 2.2. Let the corresponding partial Ritz matrix be given by $Y_\theta \equiv Q_k S_\theta$. Let $\mathscr{A}_k(\theta, z)$ and $\mathscr{A}_{l+1:k}(\theta, z)$ denote the bivariate adjugate polynomials defined above.*

Then

$$\operatorname{vec}(Y_\theta) = \begin{pmatrix} \mathscr{A}_k(\theta, A) \\ \mathscr{A}'_k(\theta, A) \\ \vdots \\ \dfrac{\mathscr{A}^{(\alpha-1)}_k(\theta, A)}{(\alpha-1)!} \end{pmatrix} q_1 + \sum_{l=1}^{k} c_{1:l-1} \begin{pmatrix} \mathscr{A}_{l+1:k}(\theta, A) \\ \mathscr{A}'_{l+1:k}(\theta, A) \\ \vdots \\ \dfrac{\mathscr{A}^{(\alpha-1)}_{l+1:k}(\theta, A)}{(\alpha-1)!} \end{pmatrix} f_l, \tag{3.17}$$

where the derivation of the bivariate adjugate polynomials is to be understood with respect to the shift θ.

Proof. We know by Theorem 2.1, Eq. (2.2) that the basis vectors $\{q_j\}_{j=1}^{k}$ satisfy

$$q_j = \left(\frac{\chi_{1:j-1}(A)}{c_{1:j-1}}\right) q_1 + \sum_{l=1}^{j-1} \left(\frac{\chi_{l+1:j-1}(A)}{c_{l:j-1}}\right) f_l. \tag{3.18}$$

Using the representation

$$Y_\theta = Q_k S_\theta = \sum_{j=1}^{k} q_j e_j^{\mathrm{T}} S_\theta \tag{3.19}$$

of the partial Ritz matrix and the representation

$$e_j^{\mathrm{T}} S_\theta = c_{1:j-1} e_1^{\mathrm{T}} \chi_{j+1:k}(J_\theta) \tag{3.20}$$

of the by virtue of Lemma 2.2 chosen partial eigenmatrix S_θ we obtain

$$Y_\theta = \sum_{j=1}^{k} q_j c_{1:j-1} e_1^{\mathrm{T}} \chi_{j+1:k}(J_\theta). \tag{3.21}$$

We insert the expression (3.18) for the basis vectors into Eq. (3.21) to obtain

$$Y_\theta = \sum_{j=1}^{k} \chi_{1:j-1}(A) q_1 e_1^{\mathrm{T}} \chi_{j+1:k}(J_\theta) + \sum_{j=1}^{k} \sum_{l=1}^{j-1} c_{1:l-1} \chi_{l+1:j-1}(A) f_l e_1^{\mathrm{T}} \chi_{j+1:k}(J_\theta) \tag{3.22}$$

and make use of the alternative expression of the (trailing) shifted adjugate polynomials $\{\mathscr{A}_{l+1:k}\}_{l=0}^{k-1}$ and their derivatives with respect to θ stated in Lemma 3.5 to obtain Eq. (3.17). □

The result of Theorem 3.6 shows that, similar to the power method, in finite precision we might expect eigenvalue approximations *even* when the starting vector has no part in direction of any corresponding eigenvector. The special form of the perturbation terms might help to determine conditions explaining when in the symmetric method of Lanczos the unscaled residuals of the Ritz pairs become small after they have grown for some steps. When the trailing adjugate polynomials and the Ritz values are such that some of the polynomials $\mathscr{A}_{l+1:k}(\theta, A)$ are close to a spectral projector, the perturbation terms result in approximate eigenvectors which are not related in any way to the starting vector.

3.3. Angles

In this section we use the last result to express the matrix of angles $\hat{V}_\lambda^H Y_\theta$ between a right partial Ritz matrix Y_θ and a left partial eigenmatrix $\hat{V}_\lambda$ of A. This result, an immediate consequence of Theorem 3.6, is merely included to clarify the axes and factors of the nonlinear amplification present in the construction of the Ritz vectors.

Theorem 3.7. *Let all notations be given as in Theorem 3.6 and let $Y_\theta \equiv Q_k S_\theta$, where S_θ is the unique right eigenmatrix from Lemma 2.2.*

Then the angles between this right partial Ritz matrix Y_θ and any left partial eigenmatrix $\hat{V}_\lambda$ of A are given by

$$\operatorname{vec}(\hat{V}_\lambda^H Y_\theta) = \begin{pmatrix} \mathscr{A}_k(\theta, J_\lambda) \\ \mathscr{A}_k'(\theta, J_\lambda) \\ \vdots \\ \dfrac{\mathscr{A}_k^{(\alpha-1)}(\theta, J_\lambda)}{(\alpha-1)!} \end{pmatrix} \hat{V}_\lambda^H q_1 + \sum_{l=1}^{k} c_{1:l-1} \begin{pmatrix} \mathscr{A}_{l+1:k}(\theta, J_\lambda) \\ \mathscr{A}_{l+1:k}'(\theta, J_\lambda) \\ \vdots \\ \dfrac{\mathscr{A}_{l+1:k}^{(\alpha-1)}(\theta, J_\lambda)}{(\alpha-1)!} \end{pmatrix} \hat{V}_\lambda^H f_l. \tag{3.23}$$

Proof. The result follows by multiplication of the result (3.17) of Theorem 3.6 with any left partial eigenmatrix $\hat{V}_\lambda^H$. □

4. Linear systems: QOR

The QOR approach is used to approximately solve a linear system $Ax = r_0$ when a square matrix C_k approximating A in some sense is at hand. The QOR approach in context of Krylov subspace methods is based on the choice $q_1 = r_0/\|r_0\|$ and the prolongation $x_k \equiv Q_k z_k$ of the solution z_k of the linear system of equations

$$C_k z_k = \|r_0\| e_1. \tag{4.1}$$

A solution does only exist when C_k is regular, the solution in this case given by $z_k = C_k^{-1}\|r_0\|e_1$. We call z_k the QOR *solution* and x_k the QOR *iterate*. We need another formulation for z_k based on polynomials. We denote the Lagrange (the Hermite) interpolation polynomial that interpolates z^{-1} (and its derivatives) at the Ritz values by $\mathscr{L}_k[z^{-1}](z)$.

Lemma 4.1 (The Lagrange interpolation of the inverse). *The interpolation polynomial $\mathscr{L}_k[z^{-1}](z)$ of the function z^{-1} at the Ritz values is defined for nonsingular unreduced Hessenberg C_k, can be expressed in terms of the characteristic polynomial $\chi_k(z)$, and is given explicitly by*

$$\begin{aligned}\mathscr{L}_k[z^{-1}](z) &= \begin{cases} \dfrac{\chi_k(0)-\chi_k(z)}{\chi_k(0)} z^{-1}, & z \neq 0,\\ -\dfrac{\chi_k'(0)}{\chi_k(0)}, & z = 0,\end{cases}\\ &= -\frac{\mathscr{A}_k(0,z)}{\chi_k(0)}.\end{aligned} \tag{4.2}$$

Proof. It is easy to see that the right-hand side is a polynomial of degree $k-1$, since we explicitly remove the constant term and divide by z. Let us denote the right-hand side for the moment by p_{k-1}. By Cayley-Hamilton the polynomial evaluated at the nonsingular matrix C_k gives

$$p_{k-1}(C_k) = \frac{\chi_k(0)I - \chi_k(C_k)}{\chi_k(0)} C_k^{-1} = \frac{\chi_k(0)}{\chi_k(0)} C_k^{-1} = C_k^{-1}. \tag{4.3}$$

Thus we have found a polynomial of degree $k-1$ taking the right values at k points (counting multiplicity). The result is proven since the interpolation polynomial is unique. □

We extend the definition and notation to trailing submatrices.

Definition 4.2 (*Trailing interpolations of the inverse*). The *trailing interpolations* of the function z^{-1} are defined for nonsingular $C_{l+1:k}$ to be the interpolation polynomials $\mathscr{L}_{l+1:k}[z^{-1}](z)$ of the function z^{-1} at the Ritz values of the trailing submatrices $C_{l+1:k}$ and are given explicitly due to the preceding Lemma 4.1 by

$$\begin{aligned}\mathscr{L}_{l+1:k}[z^{-1}](z) &= \begin{cases} \dfrac{\chi_{l+1:k}(0)-\chi_{l+1:k}(z)}{\chi_{l+1:k}(0)} z^{-1}, & z \neq 0,\\ -\dfrac{\chi_{l+1:k}'(0)}{\chi_{l+1:k}(0)}, & z = 0,\end{cases}\\ &= -\frac{\mathscr{A}_{l+1:k}(0,z)}{\chi_{l+1:k}(0)}.\end{aligned} \tag{4.4}$$

We are also confronted with interpolations of the singularly perturbed identity function $1 - \delta_{z0}$, where $\delta_{z0}(z)$ is defined by

$$\delta_{z0}(z) \equiv \begin{cases} 1, & z = 0, \\ 0, & z \neq 0. \end{cases} \tag{4.5}$$

Definition 4.3 (*Interpolations of a perturbed identity*). To nonsingular $C_{l+1:k}$ we define the interpolation polynomials $\mathscr{L}^0_{l+1:k}[1-\delta_{z0}](z)$ that interpolate the identity at the Ritz values of the trailing submatrices $C_{l+1:k}$ and have an additional zero at the node 0 by

$$\mathscr{L}^0_{l+1:k}[1-\delta_{z0}] \equiv \frac{\chi_{l+1:k}(0) - \chi_{l+1:k}(z)}{\chi_{l+1:k}(0)} = \mathscr{L}_{l+1:k}[z^{-1}]z. \tag{4.6}$$

The last equality in Eq. (4.6) better reveals the characteristics to be expected from such a singular interpolation. We observe that the resulting polynomials are of degree $k-l$ and behave like $z^{k-l}/\det(C_{l+1:k})$ for z outside the field of values of $C_{l+1:k}$ and like $\chi'_{l+1:k}(0)z/\det(C_{l+1:k})$ for z close to zero. These observations help to understand how QOR Krylov subspace methods choose Ritz values.

4.1. Residuals

It is well known, see e.g. [45] that in unperturbed Krylov subspace methods the QOR residual vector r_k is related to the starting residual vector by the so-called *residual polynomial* $\mathscr{R}_k(z)$, $r_k = \mathscr{R}_k(A)r_0$, which is given by

$$\begin{aligned} \mathscr{R}_k(z) &\equiv \det(I_k - zC_k^{-1}) = \frac{\chi_k(z)}{\chi_k(0)} \\ &= 1 - z\mathscr{L}_k[z^{-1}](z) = 1 - \mathscr{L}^0_k[1-\delta_{z0}](z) \\ &= \prod_{j=1}^{k}\left(1 - \frac{z}{\theta_j}\right) = \prod_{\theta}\left(1 - \frac{z}{\theta}\right)^{\alpha(\theta)}. \end{aligned} \tag{4.7}$$

This result is a byproduct of the following result that applies to *all* abstract perturbed Krylov subspace methods captured by (1.1). The polynomials $\mathscr{R}_k$ are almost never constructed explicitly; the exact methods are just an economic means of implicit computation. Nevertheless, the computation of the *vectors* $\mathscr{R}_k(A)r_0$ might be considered of interest when we consider perturbed methods; unfortunately, there is no easy way to update these vectors directly as the polynomials $\mathscr{R}_k$ can not be updated easily from one step to the next.

Theorem 4.4 (The QOR residual vectors). *Suppose a perturbed Krylov decomposition* (1.1) *is given with* $q_1 = r_0/\|r_0\|$. *Suppose that* C_k *is invertible such that the QOR approach can be applied. Let* x_k *denote the QOR iterate and* $r_k = r_0 - Ax_k$ *the corresponding residual.*

Then

$$r_k = \mathscr{R}_k(A)r_0 + \|r_0\| \sum_{l=1}^{k} c_{1:l-1} \frac{\chi_{l+1:k}(A) - \chi_{l+1:k}(0)}{\chi_{1:k}(0)} f_l. \tag{4.8}$$

Suppose further that all $C_{l+1:k}$ *are regular. Define* $\mathscr{R}_{l+1:k}(z) \equiv \chi_{l+1:k}(z)/\chi_{l+1:k}(0)$.

Then

$$\begin{aligned} r_k &= \mathscr{R}_k(A)r_0 + \sum_{l=1}^{k} z_{lk}\mathscr{L}^0_{l+1:k}[1-\delta_{z0}](A)f_l \\ &= \mathscr{R}_k(A)r_0 - \sum_{l=1}^{k} z_{lk}\mathscr{R}_{l+1:k}(A)f_l + F_k z_k. \end{aligned} \tag{4.9}$$

Remark 4.1. The last line of Eq. (4.9) is a key result to understand inexact Krylov subspace methods using the QOR approach. As long as the residual polynomials $\mathscr{R}_k$ and $\mathscr{R}_{l+1:k}$ are such that the corresponding terms decay to zero, or at least until reaching some threshold below the desired accuracy, the term $F_k z_k$ dominates the size of the reachable exact residual. This is reflected in the assumptions that the residuals become small even in the inexact methods, for the special case of the inexact CG method see [48, Section 6], compare with the remarks in [43, Section 6].

Proof. Again, our starting point is the Krylov decomposition

$$Q_k C_k - AQ_k = -q_{k+1}c_{k+1,k}e_k^{\mathrm{T}} + F_k. \tag{4.10}$$

We compute the residual by applying $z_k/\|r_0\| = C_k^{-1}e_1$ from the right,

$$\frac{r_k}{\|r_0\|} = \frac{-c_{k+1,k}z_{kk}}{\|r_0\|}q_{k+1} + \sum_{l=1}^{k}\frac{z_{lk}}{\|r_0\|}f_l. \tag{4.11}$$

We represent the inverse of $-C_k$ in terms of the adjugate and the determinant,

$$\frac{z_{lk}}{\|r_0\|} = -e_l^{\mathrm{T}}(-C_k)^{-1}e_1 = -\frac{e_l^{\mathrm{T}}\operatorname{adj}(-C_k)e_1}{\det(-C_k)} = -\frac{c_{1:l-1}\chi_{l+1:k}(0)}{\chi_k(0)}. \tag{4.12}$$

Thus,

$$\frac{r_k}{\|r_0\|} = \frac{c_{1:k}}{\chi_{1:k}(0)}q_{k+1} - \sum_{l=1}^{k}\frac{c_{1:l-1}\chi_{l+1:k}(0)}{\chi_{1:k}(0)}f_l. \tag{4.13}$$

When we insert the representation of the next basis vector from Eq. (2.2) we obtain Eq. (4.8). When $C_{l+1:k}$ is regular and thus $\chi_{l+1:k}(0) \neq 0$, the first line of Eq. (4.9) follows with Eq. (4.12),

$$\begin{aligned} c_{1:l-1}\frac{\chi_{l+1:k}(A)-\chi_{l+1:k}(0)}{\chi_{1:k}(0)} &= \left(-\frac{c_{1:l-1}\chi_{l+1:k}(0)}{\chi_{1:k}(0)}\right)\cdot\left(\frac{\chi_{l+1:k}(0)-\chi_{l+1:k}(A)}{\chi_{l+1:k}(0)}\right) \\ &= \frac{z_{lk}}{\|r_0\|}\cdot\mathscr{L}^0_{l+1:k}[1-\delta_{z0}](A), \end{aligned} \tag{4.14}$$

where we have used the definition of the interpolation of the perturbed identity from Eq. (4.6). The last line follows, since

$$\mathscr{R}_{l+1:k}(z) = 1 - z\mathscr{L}_{l+1:k}[z^{-1}](z) = 1 - \mathscr{L}^0_{l+1:k}[1-\delta_{z0}](z) \tag{4.15}$$

and thus $\mathscr{L}^0_{l+1:k} = 1 - \mathscr{R}_{l+1:k}$. $\square$

Theorem 4.4 also appears with another proof for CG in the recent paper [31, Theorem 5.3] by Meurant and Strakoš and in the new book [30, Theorem 5.6] by Meurant. The proof given here applies to the general case and is equally simple. Furthermore, the polynomials are identified with certain interpolation polynomials.

4.2. Iterates

In this section we shift our focus to the iterates $x_k = Q_k z_k$. We prove that the iterates are connected to a simple polynomial interpolation problem.

Theorem 4.5. *Suppose that C_k is regular. Define $z_k = C_k^{-1} e_1 \|r_0\|$ and denote the kth QOR iterate by $x_k \equiv Q_k z_k$.*

Then

$$x_k = \mathscr{L}_k[z^{-1}](A) r_0 - \|r_0\| \sum_{l=1}^{k} c_{1:l-1} \frac{\mathscr{A}_{l+1:k}(0, A)}{\chi_{1:k}(0)} f_l. \tag{4.16}$$

Suppose further that all $C_{l+1:k}$ are regular.

Then

$$x_k = \mathscr{L}_k[z^{-1}](A) r_0 - \sum_{l=1}^{k} z_{lk} \mathscr{L}_{l+1:k}[z^{-1}](A) f_l. \tag{4.17}$$

Remark 4.2. This proves that the kth iterate is a linear combination of $k+1$ approximations to the inverse of A obtained from distinct Krylov subspaces spanned by the same matrix A and different starting vectors, namely r_0 and $\{-z_{lk} f_l\}_{l=1}^{k}$, the latter changing in every step.

Proof. We know that $x_k = Q_k z_k = \sum_{j=1}^{k} q_j z_{jk}$. Inserting the expression for the basis vectors given in Eq. (3.18) and the expression for the elements z_{jk} of z_k given in Eq. (4.12),

$$\frac{x_k}{\|r_0\|} = -\sum_{j=1}^{k} \frac{\chi_{j-1}(A)\chi_{j+1:k}(0)}{\chi_k(0)} q_1 - \sum_{j=1}^{k}\sum_{l=1}^{j-1} \frac{c_{1:l-1}\chi_{l+1:j-1}(A)\chi_{j+1:k}(0)}{\chi_k(0)} f_l. \tag{4.18}$$

We switch the order of summation according to $\sum_{j=1}^{k}\sum_{l=1}^{j-1} = \sum_{l=1}^{k}\sum_{j=l+1}^{k}$. We insert the alternative expression of the adjugate polynomials given in Lemma 3.5,

$$\sum_{j=l+1}^{k} \chi_{l+1:j-1}(A)\chi_{j+1:k}(0) = \mathscr{A}_{l+1:k}(0, A) \quad \forall l = 0, 1, \ldots, k. \tag{4.19}$$

Thus, Eq. (4.18) simplifies further to

$$\frac{x_k}{\|r_0\|} = -\frac{\mathscr{A}_k(0, A)}{\chi_k(0)} q_1 - \sum_{l=1}^{k} c_{1:l-1} \frac{\mathscr{A}_{l+1:k}(0, A)}{\chi_k(0)} f_l. \tag{4.20}$$

Now, Eq. (4.16) follows from Eq. (4.2). Similarly to the transformation used in the case of the residuals, when $C_{l+1:k}$ is regular and thus $\chi_{l+1:k}(0) \neq 0$, by Eqs. (4.12) and (4.4),

$$\begin{aligned} c_{1:l-1} \frac{\mathscr{A}_{l+1:k}(0, A)}{\chi_k(0)} &= \left(-\frac{c_{1:l-1}\chi_{l+1:k}(0)}{\chi_k(0)}\right) \cdot \left(-\frac{\mathscr{A}_{l+1:k}(0, A)}{\chi_{l+1:k}(0)}\right) \\ &= \frac{z_{lk}}{\|r_0\|} \cdot \mathscr{L}_{l+1:k}[z^{-1}](A), \end{aligned} \tag{4.21}$$

we obtain Eq. (4.17). □

4.3. Errors

We next derive a theorem that gives an explicit expression for the error vectors $x - x_k$.

Theorem 4.6 (The QOR error vectors). *Suppose a perturbed Krylov decomposition* (1.1) *is given with* $q_1 = r_0/\|r_0\|$. *Suppose that* C_k *is invertible such that the QOR approach can be applied. Let* x_k *denote the QOR iterate and* $r_k = r_0 - Ax_k$ *the corresponding residual. Suppose further that* A *is invertible and let* $x = A^{-1}r_0$ *denote the unique solution of the linear system* $Ax = r_0$.

Then

$$(x - x_k) = \mathscr{R}_k(A)(x - o) + \|r_0\| \sum_{l=1}^{k} c_{1:l-1} \frac{\mathscr{A}_{l+1:k}(0, A)}{\chi_{1:k}(0)} f_l. \tag{4.22}$$

Suppose further that all trailing submatrices $C_{l+1:k}$, $l = 1, \ldots, k-1$ *are nonsingular.*

Then

$$\begin{aligned}(x - x_k) &= \mathscr{R}_k(A)(x - o) + \sum_{l=1}^{k} z_{lk} \mathscr{L}_{l+1:k}[z^{-1}](A) f_l \\ &= \mathscr{R}_k(A)(x - o) - \sum_{l=1}^{k} z_{lk} \mathscr{R}_{l+1:k}[z^{-1}](A) A^{-1} f_l + A^{-1} F_k z_k.\end{aligned} \tag{4.23}$$

Proof. The results (4.22) and (4.23) follow by subtracting both sides of Eq. (4.16) and the first line of Eq. (4.17) from the trivial equation $x = x$ and the observation that $\mathscr{L}_k(z) = (1 - \mathscr{R}_k[z^{-1}](z))z^{-1}$. The last line uses the similar transformations $\mathscr{L}_{l+1:k}(z) = (1 - \mathscr{R}_{l+1:k}[z^{-1}](z))z^{-1}$ to express the error terms in residual form, which results in the additional term $+A^{-1}F_k z_k$. $\square$

5. Linear systems: QMR

Most part of this section is based on rewriting well known results, e.g. [18,9,42,29,48], using the language of polynomials. This has been done in part already in the previous note [51]. Even though most of the material is thus known, for better accessibility we include short proofs more or less equal to the known ones adapted to the polynomial language. We remark that the polynomial versions of the results are slightly more complicated, but they seem necessary to derive the theorems in this section. These resulting theorems are believed to be new, at least in the non-exact case.

The QMR approach is used to approximately solve a linear system $A\underline{x} = \underline{r}_0$ when a *rectangular* approximation to A is at hand. To better distinguish the QMR approach from the QOR approach we denote the starting residual by $\underline{r}_0$ instead of r_0 and the solution by $\underline{x}$ instead of x. Mostly, $\underline{r}_0 \equiv r_0$ and thus $\underline{x} = x$. The QMR approach in context of Krylov subspace methods is based on the choice $q_1 = \underline{r}_0/\|\underline{r}_0\|$ and the prolongation $\underline{x}_k \equiv Q_k \underline{z}_k$ of the solution $\underline{z}_k$ of the least-squares problem

$$\|\underline{C}_k \underline{z}_k - \|\underline{r}_0\| \underline{e}_1\| = \min. \tag{5.1}$$

We call $\underline{z}_k$ the QMR *solution* and $\underline{x}_k$ the QMR *iterate*. Since $\underline{C}_k$ is extended unreduced Hessenberg, obviously $\underline{C}_k$ has full rank k. By definition of $\check{\underline{\nu}}$ and [51, Lemma 3.1, Eq. (3.5)], already proven in [18, Eqs. (3.4) and (3.8)] and used in [48], the extended nonzero vector $\check{\underline{\nu}}(0)^{\mathrm{T}}$ spans the left null space of $\underline{C}_k$,

$$\check{\underline{\nu}}(0)^{\mathrm{T}}\underline{C}_k = \hat{\underline{\nu}}(0)^H\underline{C}_k = o_k^{\mathrm{T}}. \tag{5.2}$$

The unique solution $\underline{z}_k$ of the least-squares problem (5.1) and its residual $\mathfrak{r}_k$ are given by

$$\underline{z}_k \equiv \|\underline{r}_0\|\underline{C}_k^{\dagger}\underline{e}_1, \quad \mathfrak{r}_k \equiv \underline{e}_1\|\underline{r}_0\| - \underline{C}_k\underline{z}_k = \|\underline{r}_0\|(I_{k+1} - \underline{C}_k\underline{C}_k^{\dagger})\underline{e}_1. \tag{5.3}$$

We call the residual $\mathfrak{r}_k$ of the Hessenberg least-squares problem (5.1) the *quasi-residual* of the linear system $A\underline{x} = \underline{r}_0$. The residual $\underline{r}_k$ of the QMR approximation $\underline{x}_k \equiv Q_k\underline{z}_k$ is related to the quasi-residual as follows:

$$\begin{aligned} \underline{r}_k &= \underline{r}_0 - A\underline{x}_k = Q_{k+1}\underline{e}_1\|\underline{r}_0\| - AQ_k\underline{z}_k \\ &= Q_{k+1}(\underline{e}_1\|\underline{r}_0\| - \underline{C}_k\underline{z}_k) + F_k\underline{z}_k = Q_{k+1}\mathfrak{r}_k + \sum_{l=1}^{k} f_l\underline{z}_{lk}. \end{aligned} \tag{5.4}$$

To proceed, we construct another expression for the least-squares solution $\underline{z}_k$ and the quasi-residual $\mathfrak{r}_k$ revealing the dependency from characteristic polynomials involving submatrices of $\underline{C}_k$, compare with the similar but simpler expressions [42, Proposition 4.1], [29, Theorem 2.1] and [48, Lemma 2.2].

Lemma 5.1 (The vectors $\underline{z}_k$ and $\mathfrak{r}_k$). *Let $\underline{C}_k \in \mathbb{C}^{(k+1)\times k}$ be an unreduced extended upper Hessenberg matrix. Let $C_{k+1}^{\Delta} \in \mathbb{C}^{k\times k}$ denote the regular upper triangular matrix $\underline{C}_k$ without its first row.*

Then the elements of the inverse of C_{k+1}^{Δ} are given by

$$((C_{k+1}^{\Delta})^{-1})_{lj} = \begin{cases} \dfrac{\chi_{l+1:j}(0)}{c_{l:j}}, & l \leqslant j, \\ 0, & l > j, \end{cases} \tag{5.5}$$

the vectors $\underline{z}_k$ and $\mathfrak{r}_k$ by

$$\frac{\underline{z}_k}{\|\underline{r}_0\|} = \begin{pmatrix} o_k & -(C_{k+1}^{\Delta})^{-1} \end{pmatrix} \frac{\hat{\underline{\nu}}(0)}{\|\check{\underline{\nu}}(0)\|^2} \quad \textit{and} \quad \frac{\mathfrak{r}_k}{\|\underline{r}_0\|} = \frac{\hat{\underline{\nu}}(0)}{\|\check{\underline{\nu}}(0)\|^2}. \tag{5.6}$$

Proof. The expression for the inverse follows by the representation as adjugate by determinant, compare with [51, Lemma 3.4]. The nonzero vector $\hat{\underline{\nu}}(0)^H$ spans the left null space and $\underline{C}_k$ has full rank k. Thus, the matrix $\underline{C}_k\underline{C}_k^{\dagger}$ is given by

$$\underline{C}_k\underline{C}_k^{\dagger} = I_{k+1} - \frac{\hat{\underline{\nu}}(0)\hat{\underline{\nu}}(0)^H}{\|\check{\underline{\nu}}(0)\|^2}. \tag{5.7}$$

By definition of $\mathfrak{r}_k$, Eq. (5.3), and since $\hat{\nu}_1(0) = 1$, the quasi-residual is given by the expression in Eq. (5.6). The relation $\mathfrak{r}_k = \underline{e}_1\|\underline{r}_0\| - \underline{C}_k\underline{z}_k$ can be embedded into

$$\begin{aligned} \begin{pmatrix} \underline{e}_1 & -\underline{C}_k \end{pmatrix} \begin{pmatrix} 0 \\ \underline{z}_k \end{pmatrix} &= \mathfrak{r}_k - \underline{e}_1\|\underline{r}_0\| \\ \Leftrightarrow \quad \begin{pmatrix} 0 \\ \underline{z}_k \end{pmatrix} &= \begin{pmatrix} 1 & c_{1,1:k}(C_{k+1}^{\Delta})^{-1} \\ o_k & -(C_{k+1}^{\Delta})^{-1} \end{pmatrix} (\mathfrak{r}_k - \underline{e}_1\|\underline{r}_0\|). \end{aligned} \tag{5.8}$$

We remove the first column and use the fact that $\underline{e}_1$ is in the null space of the matrix with $(C_{k+1}^{\Delta})^{-1}$ in its lower block to obtain the expression for $\underline{z}_k$ in Eq. (5.6). $\square$

When all leading submatrices C_j are regular, which is the case, e.g. in the unperturbed CG method applied to a symmetric positive definite matrix $A \in \mathbb{R}^{n\times n}$, we can rewrite part of the results of Lemma 5.1 in terms of the QOR quantities. The next lemma states that the QMR solution (iterate) is a convex combination of all prior QOR solutions (iterates). Together with the resulting properties of the corresponding residuals this is a well-known fact, see e.g. [6,9] and for general relations in the context of OR and MR methods [16]. To proceed, we explicitly need the special structure of the coefficients of this convex combination.

Lemma 5.2 (The relation between $\underline{z}_k$ and z_j, $j \leqslant k$). *Suppose that all leading C_j, $j = 1, \ldots, k$ are regular and that $r_0 \equiv \underline{r}_0$.*

Then

$$\underline{z}_k = \frac{\sum_{j=0}^k |\check{\nu}_{j+1}(0)|^2 \begin{pmatrix} z_j \\ o_{k-j} \end{pmatrix}}{\|\check{\underline{\nu}}(0)\|^2}, \quad \underline{x}_k = \frac{\sum_{j=0}^k |\check{\nu}_{j+1}(0)|^2 x_j}{\|\check{\underline{\nu}}(0)\|^2}, \tag{5.9}$$

where for convenience we interpret z_0 as the empty matrix with dimensions 0×1.

Remark 5.1. The representation of QOR solutions and QOR iterates with interpolation polynomials suggests a representation of the polynomials associated with the QMR approach as convex combinations of all corresponding prior QOR polynomials. Because of the close relations, the same holds true for the associated residual and perturbed identity polynomials. We seek the coefficients such that this relationship gives rise to a definition of the polynomials associated with QMR *independent* of the existence of the QOR polynomials.

Proof. The jth QOR solution z_j can be embedded into

$$\begin{aligned}(\underline{e}_1 \quad -\underline{C}_k)\begin{pmatrix} 0 \\ z_j \\ o_{k-j}\end{pmatrix} &= -c_{j+1,j} z_{jj} e_{j+1} - \underline{e}_1\|\underline{r}_0\| = \frac{c_{1:j}}{\chi_{1:j}(0)} e_{j+1} - \underline{e}_1\|\underline{r}_0\| \\ &= \frac{1}{\check{\nu}_{j+1}(0)} e_{j+1} - \underline{e}_1\|\underline{r}_0\|.\end{aligned} \tag{5.10}$$

Multiplication by $|\check{\nu}_{j+1}(0)|^2$, summation over j and division by $\|\check{\underline{\nu}}(0)\|^2$ results in

$$\left(\underline{e}_1 \quad -\underline{C}_k\right) \frac{\sum_{j=0}^k |\check{\nu}_{j+1}(0)|^2 \begin{pmatrix} 0 \\ z_j \\ o_{k-j}\end{pmatrix}}{\|\check{\underline{\nu}}(0)\|^2} = \frac{\hat{\underline{\nu}}(0)}{\|\check{\underline{\nu}}(0)\|^2} - \underline{e}_1\|\underline{r}_0\|. \tag{5.11}$$

The matrix $\left(\underline{e}_1 \quad -\underline{C}_k\right)$ is regular, which proves the first part of Eq. (5.9) by comparison of Eq. (5.11) with Eq. (5.8). The second part of Eq. (5.9) follows upon multiplication by Q_k from the left. □

This indicates how the residual and other polynomials associated with the QMR approach might be constructed. The expressions given in the following apply also to cases where the submatrices C_j are not necessarily regular.

Definition 5.3 (*The polynomials $\underline{\mathscr{R}}_k$, $\underline{\mathscr{L}}_k$ and $\underline{\mathscr{L}}_k^0$*). We define the polynomials $\underline{\mathscr{R}}_k(z)$, $\underline{\mathscr{L}}_k[z^{-1}](z)$ and $\underline{\mathscr{L}}_k^0[1-\delta_{z0}](z)$ by

$$\underline{\mathscr{R}}_k(z) \equiv \frac{\sum_{j=1}^{k+1} \hat{\nu}_j(0)\check{\nu}_j(z)}{\|\check{\underline{\nu}}(0)\|^2}, \tag{5.12}$$

$$\underline{\mathscr{L}}_k[z^{-1}](z) \equiv \frac{\sum_{j=1}^{k+1} \hat{\nu}_j(0)(c_{1:j-1})^{-1}(-\mathscr{A}_{j-1}(0,z))}{\|\check{\underline{\nu}}(0)\|^2}, \tag{5.13}$$

$$\underline{\mathscr{L}}_k^0[1-\delta_{z0}](z) \equiv \frac{\sum_{j=1}^{k+1} \hat{\nu}_j(0)(\check{\nu}_j(0)-\check{\nu}_j(z))}{\|\check{\underline{\nu}}(0)\|^2}. \tag{5.14}$$

With these definitions,

$$\begin{aligned}
&\underline{\mathscr{R}}_k(z) = 1 - \underline{\mathscr{L}}_k^0[1-\delta_{z0}](z) = 1 - z\underline{\mathscr{L}}_k[z^{-1}](z),\\
&\deg(\underline{\mathscr{R}}_k(z)) = \deg(\underline{\mathscr{L}}_k^0[1-\delta_{z0}](z)) = \deg(\underline{\mathscr{L}}_k[z^{-1}](z)) + 1.
\end{aligned} \tag{5.15}$$

When all C_j are regular, by inspection

$$\underline{\mathscr{R}}_k(z) = \frac{\sum_{j=0}^{k} |\check{\nu}_{j+1}(0)|^2 \mathscr{R}_j(z)}{\|\check{\underline{\nu}}(0)\|^2}, \tag{5.16}$$

$$\underline{\mathscr{L}}_k[z^{-1}](z) = \frac{\sum_{j=0}^{k} |\check{\nu}_{j+1}(0)|^2 \mathscr{L}_j[z^{-1}](z)}{\|\check{\underline{\nu}}(0)\|^2}, \tag{5.17}$$

$$\underline{\mathscr{L}}_k^0[1-\delta_{z0}](z) = \frac{\sum_{j=0}^{k} |\check{\nu}_{j+1}(0)|^2 \mathscr{L}_j^0[1-\delta_{z0}](z)}{\|\check{\underline{\nu}}(0)\|^2}. \tag{5.18}$$

To better understand the *interpolation* properties of the polynomials defined in Definition 5.3 we need another expression for the residual polynomial that gives more insight. To obtain this expression, we need the following auxiliary simple lemma.

Lemma 5.4. *Suppose that $A \in \mathbb{C}^{n\times n}$ is given. Let A_{n-1} denote its leading principal submatrix consisting of the columns and rows indexed from 1 to $n-1$.*
Then

$$\det(A + z e_n e_n^{\mathrm{T}}) = \det(A) + z\det(A_{n-1}). \tag{5.19}$$

Proof. Eq. (5.19) follows from the multilinearity of the determinant. □

We define the characteristic matrix of $\underline{C}_k$ by ${}^z\underline{C}_k \equiv z\underline{I}_k - \underline{C}_k$. In the sequel we need some knowledge about matrices of the form $-\underline{C}_k^{H\,z}\underline{C}_k$ expressed in terms of rank-one modified square matrices. It is easy to see that

$$-\underline{C}_k^{H\,z}\underline{C}_k = \begin{pmatrix} -C_k \\ -c_{k+1,k}e_k^{\mathrm{T}} \end{pmatrix}^H \begin{pmatrix} {}^zC_k \\ -c_{k+1,k}e_k^{\mathrm{T}} \end{pmatrix} = -C_k^{H\,z}C_k + |c_{k+1,k}|^2 e_k e_k^{\mathrm{T}}. \tag{5.20}$$

We need the leading principal submatrix of size $(k-1)\times(k-1)$ of $C_k^{H\,z}C_k$, denoted by $(C_k^{H\,z}C_k)_{k-1}$. Obviously,

$$(C_k^{H\,z}C_k)_{k-1} = \underline{C}_{k-1}^{H\,z}\underline{C}_{k-1}. \tag{5.21}$$

Now we can characterize the so-called *quasi-kernel polynomials* $\underline{\mathscr{R}}_k(z)$ further in the following lemma, compare with [18, Theorem 3.2, Corollary 5.3].

Lemma 5.5 (The quasi-kernel polynomials). *Let* ${}^{z}\underline{C}_k \equiv z\underline{I}_k - \underline{C}_k$ *denote the characteristic matrix of* $\underline{C}_k$ *and define* ${}^{0}\underline{C}_k \equiv -\underline{C}_k$. *Let letter* μ *denote the eigenvalues of the generalized eigenvalue problem*

$$C_k^H u = \mu \underline{C}_k^H \underline{C}_k u \tag{5.22}$$

and let letter $\vartheta = 1/\mu$ *denote the eigenvalues of the generalized eigenvalue problem*

$$\underline{C}_k^H \underline{C}_k u = \vartheta C_k^H u, \tag{5.23}$$

where the algebraic multiplicity of μ *and* ϑ *is denoted by* $\alpha(\mu)$ *and* $\alpha(\vartheta)$, *respectively.*

Then

$$\begin{aligned}\underline{\mathscr{R}}_k(z) &\equiv \frac{\sum_{j=1}^{k+1} \hat{\nu}_j(0)\check{\nu}_j(z)}{\sum_{j=1}^{k+1} \hat{\nu}_j(0)\check{\nu}_j(0)} = \frac{\underline{\check{\nu}}(0)^H \underline{\check{\nu}}(z)}{\underline{\check{\nu}}(0)^H \underline{\check{\nu}}(0)} = \frac{\underline{\check{\nu}}(0)^H \underline{\check{\nu}}(z)}{\|\underline{\check{\nu}}(0)\|^2} = \frac{\det(\underline{C}_k^H {}^{z}\underline{C}_k)}{\det(\underline{C}_k^H {}^{0}\underline{C}_k)}\\ &= \frac{\det(\underline{C}_k^H \underline{C}_k - zC_k^H)}{\det(\underline{C}_k^H \underline{C}_k)} = \det(I_k - z\underline{C}_k^{\dagger}\underline{I}_k)\\ &= \prod_{\mu}(1 - z\mu)^{\alpha(\mu)} = \prod_{\vartheta}\left(1 - \frac{z}{\vartheta}\right)^{\alpha(\vartheta)}.\end{aligned} \tag{5.24}$$

Proof. We only need to prove the equation

$$\frac{\sum_{j=1}^{k+1} \hat{\nu}_j(0)\check{\nu}_j(z)}{\sum_{j=1}^{k+1} \hat{\nu}_j(0)\check{\nu}_j(0)} = \frac{\det(\underline{C}_k^H {}^{z}\underline{C}_k)}{\det(\underline{C}_k^H {}^{0}\underline{C}_k)} = \frac{\det(-\underline{C}_k^H {}^{z}\underline{C}_k)}{\det(-\underline{C}_k^H {}^{0}\underline{C}_k)}, \tag{5.25}$$

since the remaining parts of Eq. (5.24) consist of trivial rewritings. By iterated application of Lemma 5.4 and Eqs. (5.20) and (5.21),

$$\begin{aligned}\det(-\underline{C}_k^H {}^{z}\underline{C}_k) &= \det(-C_k^H {}^{z}C_k) + |c_{k+1,k}|^2 \det(-\underline{C}_{k-1}^H {}^{z}\underline{C}_{k-1})\\ &= \sum_{j=0}^{k} |c_{j+1:k}|^2 \overline{\chi_j(0)}\chi_j(z) = |c_{1:k}|^2 \sum_{j=1}^{k+1} \hat{\nu}_j(0)\check{\nu}_j(z).\end{aligned} \tag{5.26}$$

Similarly,

$$\det(-\underline{C}_k^H {}^{0}\underline{C}_k) = |c_{1:k}|^2 \sum_{j=1}^{k+1} \hat{\nu}_j(0)\check{\nu}_j(0). \tag{5.27}$$

Thus we have proven Eq. (5.25). □

In the following, we focus on the similarities and differences of the residual polynomials $\mathscr{R}_k$ and $\underline{\mathscr{R}}_k$. To reveal the similarity, we state once again the following two akin expressions for the residual polynomials,

$$\underline{\mathscr{R}}_k(z) = \det(I_k - z\underline{C}_k^{\dagger}\underline{I}_k) \quad \text{and} \quad \mathscr{R}_k(z) = \det(I_k - zC_k^{-1}). \tag{5.28}$$

The residual polynomials $\mathscr{R}_k$ cease to exist when C_k is singular, the residual polynomials $\underline{\mathscr{R}}_k$ do always exist since by assumption $\underline{C}_k$ always has full rank k. When the polynomials $\mathscr{R}_k$ exist they are of exact degree k. The degree of $\underline{\mathscr{R}}_k$ might be $k - r$ for any r in $\{0, \ldots, k\}$. As was shown in [18], non-existence of the last r residual polynomials $\mathscr{R}_j$ causes the drop in the degree of $\underline{\mathscr{R}}_k$.

The inverses $\vartheta \equiv 1/\mu$ of the eigenvalues μ (counting multiplicity) are the so-called *harmonic Ritz values*, [32,18,36]. The harmonic Ritz values are the eigenvalues of the generalized eigenvalue problem $\vartheta C_k^H u = \underline{C}_k^H \underline{C}_k u$. There are precisely $k - \alpha(\infty)$ finite eigenvalues, the infinite eigenvalues case the rank-drop. The name follows from their interpretation as harmonic mean to eigenvalues of A [36]. In the general case these values are *not* harmonic Ritz values of A, but of all $C_{k+\ell}$, $\ell \in \mathbb{N}$.

5.1. Residuals

It is known, see e.g. [18], that in unperturbed QMR Krylov subspace methods the residual vector $\underline{r}_k$ is related to the starting residual vector by $\underline{r}_k = \underline{\mathscr{R}}_k(A)\underline{r}_0$. This result for the unperturbed methods is a byproduct of the following result that applies to *all* abstract perturbed Krylov subspace methods captured by (1.1). We use the expression for the residuals $\underline{r}_k$, the representation of the basis vectors $\{q_j\}_{j=1}^{k+1}$ and the representation of the quasi-residual $\mathfrak{r}_k$ and the vector $\underline{z}_k$ in terms of polynomials to prove the following theorem.

Theorem 5.6 (The QMR residual vectors). *Suppose a perturbed Krylov decomposition* (1.1) *is given with $q_1 = \underline{r}_0/\|\underline{r}_0\|$. Let $\underline{x}_k = Q_k\underline{z}_k$ denote the QMR iterate and $\underline{r}_k = \underline{r}_0 - A\underline{x}_k$ the corresponding residual.*

Then

$$\underline{r}_k = \underline{\mathscr{R}}_k(A)\underline{r}_0 + \frac{\|\underline{r}_0\|}{\|\check{\underline{\nu}}(0)\|^2}\sum_{l=1}^{k}\left(\sum_{j=l}^{k}\hat{\nu}_{j+1}(0)\frac{\chi_{l+1:j}(A) - \chi_{l+1:j}(0)}{c_{l:j}}\right) f_l. \tag{5.29}$$

Proof. We use the expression for the residual given in Eq. (5.4),

$$\underline{r}_k = Q_{k+1}\mathfrak{r}_k + \sum_{l=1}^{k} f_l \underline{z}_{lk} = \sum_{j=1}^{k+1} q_j \mathfrak{r}_{jk} + \sum_{l=1}^{k} f_l \underline{z}_{lk}. \tag{5.30}$$

and insert the expression (5.6) for the quasi-residual $\mathfrak{r}_k$ and the solution $\underline{z}_k$ of the least-squares problem obtained in Lemma 5.1. We already have noted that by Theorem 2.1 the basis vectors $\{q_j\}_{j=1}^{k}$ are given by Eq. (3.18),

$$q_j = \left(\frac{\chi_{1:j-1}(A)}{c_{1:j-1}}\right) q_1 + \sum_{l=1}^{j-1}\left(\frac{\chi_{l+1:j-1}(A)}{c_{l:j-1}}\right) f_l. \tag{5.31}$$

Putting pieces together results in

$$\begin{aligned}
\underline{r}_k &= \underline{\mathscr{R}}_k(A)\underline{r}_0 + \frac{\|\underline{r}_0\|}{\|\check{\underline{\nu}}(0)\|^2}\sum_{j=1}^{k+1}\sum_{l=1}^{j-1}\hat{\nu}_j(0)\frac{\chi_{l+1:j-1}(A)}{c_{l:j-1}} f_l \\
&\quad + \frac{\|\underline{r}_0\|}{\|\check{\underline{\nu}}(0)\|^2} F_k \left(o_k \quad -(C_{k+1}^{\Delta})^{-1}\right)\hat{\underline{\nu}}(0) \\
&= \underline{\mathscr{R}}_k(A)\underline{r}_0 + \frac{\|\underline{r}_0\|}{\|\check{\underline{\nu}}(0)\|^2}\sum_{j=0}^{k}\sum_{l=1}^{j}\hat{\nu}_{j+1}(0)\frac{\chi_{l+1:j}(A) - \chi_{l+1:j}(0)}{c_{l:j}} f_l,
\end{aligned} \tag{5.32}$$

Switching the order of summation according to $\sum_{j=0}^{k}\sum_{l=1}^{j} = \sum_{l=1}^{k}\sum_{j=l}^{k}$ results in Eq. (5.29). □

5.2. Iterates

Inserting the by virtue of Theorem 2.1 known expressions of the basis vectors $\{q_j\}_{j=1}^{k}$ and the explicit expression for the QMR solutions $\underline{z}_k$ into the defining relation $\underline{x}_k = Q_k \underline{z}_k$ we can prove the following theorem.

Theorem 5.7 (The QMR iterates). *Suppose a perturbed Krylov decomposition* (1.1) *is given with* $q_1 = \underline{r}_0/\|\underline{r}_0\|$. *Let* $\underline{x}_k = Q_k \underline{z}_k$ *denote the kth QMR iterate.*
Then

$$\underline{x}_k = \underline{\mathscr{L}}_k[z^{-1}](A)\underline{r}_0 + \frac{\|\underline{r}_0\|}{\|\check{\underline{\nu}}(0)\|^2}\sum_{l=1}^{k}\left(\sum_{j=l}^{k}\hat{\nu}_{j+1}(0)\frac{-\mathscr{A}_{l+1:j}(0,A)}{c_{l:j}}\right) f_l. \tag{5.33}$$

Proof. We use Eq. (5.31) to obtain

$$\begin{aligned}\frac{\underline{x}_k}{\|r_0\|} &= Q_k\frac{\underline{z}_k}{\|r_0\|} = \sum_{\ell=1}^{k} q_\ell \frac{\underline{z}_{\ell k}}{\|r_0\|}\\ &= \sum_{\ell=1}^{k}\left(\left(\frac{\chi_{1:\ell-1}(A)}{c_{1:\ell-1}}\right)q_1 + \sum_{l=1}^{\ell-1}\left(\frac{\chi_{l+1:\ell-1}(A)}{c_{l:\ell-1}}\right)f_l\right)\frac{\underline{z}_{\ell k}}{\|r_0\|}\end{aligned} \tag{5.34}$$

By application of Lemma 5.1, Eqs. (5.5) and (5.6), we can write the elements $\underline{z}_{\ell k}$ of the vector $\underline{z}_k$ in the form

$$\frac{\underline{z}_{\ell k}}{\|\underline{r}_0\|} = \sum_{j=\ell}^{k}\frac{-\chi_{\ell+1:j}(0)}{c_{\ell:j}}\frac{\hat{\nu}_{j+1}(0)}{\|\check{\underline{\nu}}(0)\|^2}. \tag{5.35}$$

Thus, by switching the order of summation and the alternate description of the adjugate polynomials given in Lemma 3.5, Eq. (3.15),

$$\begin{aligned}\frac{\|\check{\underline{\nu}}(0)\|^2}{\|\underline{r}_0\|}\underline{x}_k &= \sum_{\ell=1}^{k}\sum_{j=\ell}^{k}\left(\frac{\chi_{1:\ell-1}(A)}{c_{1:\ell-1}}q_1 + \sum_{l=1}^{\ell-1}\frac{\chi_{l+1:\ell-1}(A)}{c_{l:\ell-1}}f_l\right)\frac{-\chi_{\ell+1:j}(0)}{c_{\ell:j}}\hat{\nu}_{j+1}(0)\\ &= \sum_{\ell=1}^{k}\sum_{j=\ell}^{k}\frac{\chi_{1:\ell-1}(A)}{c_{1:\ell-1}}\cdot\frac{-\chi_{\ell+1:j}(0)}{c_{\ell:j}}\hat{\nu}_{j+1}(0)q_1\\ &\quad+\sum_{\ell=1}^{k}\sum_{j=\ell}^{k}\sum_{l=1}^{\ell-1}\frac{\chi_{l+1:\ell-1}(A)}{c_{l:\ell-1}}\cdot\frac{-\chi_{\ell+1:j}(0)}{c_{\ell:j}}\hat{\nu}_{j+1}(0)f_l\\ &= \sum_{j=1}^{k}\left(\sum_{\ell=1}^{j}\frac{\chi_{1:\ell-1}(A)}{c_{1:\ell-1}}\cdot\frac{-\chi_{\ell+1:j}(0)}{c_{\ell:j}}\right)\hat{\nu}_{j+1}(0)q_1\end{aligned}$$

$$+\sum_{l=1}^{k-1}\sum_{j=l}^{k}\left(\sum_{\ell=l+1}^{j}\frac{\chi_{l+1:\ell-1}(A)}{c_{l:\ell-1}}\cdot\frac{-\chi_{\ell+1:j}(0)}{c_{\ell:j}}\right)\hat{\nu}_{j+1}(0)f_l$$

$$=\sum_{j=1}^{k}\hat{\nu}_{j+1}(0)\frac{-\mathscr{A}_j(0,A)}{c_{1:j}}q_1+\sum_{l=1}^{k-1}\left(\sum_{j=l}^{k}\hat{\nu}_{j+1}(0)\frac{-\mathscr{A}_{l+1:j}(0,A)}{c_{l:j}}\right)f_l. \tag{5.36}$$

We multiply by $\|\underline{r}_0\|/\|\check{\underline{\nu}}(0)\|^2$ and insert $\underline{\mathscr{L}}_k[z^{-1}](z)$ from its definition in Eq. (5.13). Eq. (5.33) follows since by definition $\mathscr{A}_{k+1:k}\equiv 0$. □

5.3. Errors

We define $\underline{x}\equiv A^{-1}\underline{r}_0$. We can use both the theorem on the residuals and the theorem on the iterates to obtain the following expression for the errors $\underline{x}-\underline{x}_k$.

Theorem 5.8 (The QMR error vectors). *Suppose a perturbed Krylov decomposition* (1.1) *is given with $q_1=\underline{r}_0/\|\underline{r}_0\|$. Let $\underline{x}_k=Q_k\underline{z}_k$ denote the kth QMR iterate and define $\underline{x}\equiv A^{-1}\underline{r}_0$. Then*

$$\underline{x}-\underline{x}_k=\underline{\mathscr{R}}_k(A)(\underline{x}-o)+\frac{\|\underline{r}_0\|}{\|\check{\underline{\nu}}(0)\|^2}\sum_{l=1}^{k}\left(\sum_{j=l}^{k}\hat{\nu}_{j+1}(0)\frac{\mathscr{A}_{l+1:j}(0,A)}{c_{l:j}}\right)f_l. \tag{5.37}$$

Proof. We start with $\underline{x}=\underline{x}$ and subtract Eq. (5.33). We group the leading terms and use the identity

$$\underline{\mathscr{R}}_k(A)(\underline{x}-o)=(I-\underline{\mathscr{L}}_k[z^{-1}](A)A)\underline{x}=\underline{x}-\underline{\mathscr{L}}_k[z^{-1}](A)\underline{r}_0. \tag{5.38}$$

This results in Eq. (5.37). □

6. Conclusion and outlook

We have successfully applied the Hessenberg eigenvalue–eigenmatrix relations derived in [51] to abstract perturbed Krylov subspace methods. The investigation carried out in this paper sheds some light on the methods and introduces a new point of view. This new abstract point of view on perturbed Krylov subspace methods enables no detailed convergence analysis but unifies important parts of the analysis considerably. In this abstract setting, without any additional knowledge on the properties of the computed matrices $C_k(\underline{C}_k)$, we cannot make any statements on the convergence of, say, the Ritz *values*, but the convergence of the Ritz *vectors* and the QOR iterates can be described independently of the particular method under investigation in terms of the unknown Ritz values. Even though we cannot compute bounds on the distance of the eigenvalues and the computed Ritz values, Theorem 2.3 clearly reveals that in case of random errors the Ritz values can only accidentally come arbitrarily close to the eigenvalues of A and that the occurrence of multiple Ritz values is extremely unlikely.

At least in the opinion of the author, the main achievement of the paper lies not in working out the polynomial structure presented in the results, which follows easily using basic linear algebra techniques, but in devising the deeper understanding of most of the polynomials involved and their close connection to approximation problems. In this sense the author has failed with respect to the polynomials amplifying the perturbation terms in the theorems related to the QMR case.

The results are not usable 'as is', but numerical experiments carried out by the author suggest that the leading terms based on the computed Hessenberg matrix C_k in some cases govern the convergence behavior of the corresponding methods until the maximal attainable accuracy has been reached. When one can prove for a concrete method that this is indeed the case, the convergence analysis of these methods 'simplifies' to a convergence analysis of the Ritz values of the underlying perturbed Krylov decomposition. In case of the methods based on the QMR approach this again implies a failure of the analysis given.

Missing, mainly for reasons of space, is the application of the results to a single instance of a Krylov subspace method, which may be in the form of the derivation of bounds, backward errors, convergence theorems or the stabilization of existing algorithms or even the development of entirely new methods based on the abstract insights given here. The author is currently working out the detailed application of the results to the symmetric finite precision algorithm of Lanczos; any help is appreciated.

The generalization of the approach of abstraction to Krylov subspace methods *not* covered by Eq. (1.1) must be based on a corresponding generalization of the underlying results on Hessenberg matrices. A typical and interesting candidate for such a generalization would be similar results for block Hessenberg matrices, which would allow to treat block Krylov subspace methods in a similar fashion. The author doubts that the analysis developed in [51] could easily be adopted.

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